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**WORLD ASSOCIATION
OF THEORETICAL AND
COMPUTATIONAL
CHEMISTS**

Santiago de Compostela (SPAIN)
17-22 July, 2011

posters

POSTER SESSION I

POSTER SESSION II

POSTER SESSION III

POSTER SESSION I (PI-1 to PI-283)
Sunday, July 17 - 15.30-17.30h (Faculty of Economy)

- PI-001. Flores-Holguín, Norma
Conceptual DFT study of nanomaterials for molecular and organic photovoltaics
- PI-002. Gryn'ova, Ganna
Revising the Mechanism of Polymer Autooxidation
- PI-003. Schmidt, Michael
Hydrazine decomposition mechanism
- PI-004. Prosmiiti, Rita
Theoretical study of small H_{2n+1} clusters: potential surfaces and direct dynamics simulations
- PI-005. Navizet, Isabelle
Light emission in firefly: a theoretical approach
- PI-006. Martín, Ana
Origin of the acidity enhancement of CH_2CHX ($X = NH_2, PH_2, AsH_2,$ and SbH_2) derivatives by complexation with BH_3
- PI-007. Noorizadeh, Siamak
Insight into the stability of complexes from the information theory computations
- PI-008 (previous PIII-048) Blancafort, Lluís
Fulvene excited state dynamics with MCTDH: double bond isomerization
- PI-009. Sklenak, Stepan
DFT and multi-spectroscopic study of the N_2O decomposition in the absence of NO . Why does Fe-ferrierite have a superior activity with respect to Fe-ZSM-5 and Fe-beta?
- PI-010. Donald, Kelling
Tuning sigma-holes: charge redistribution in the heavy analogues of simple and mixed halomethanes can impose strong propensities for halogen bonding
- PI-011. Jørgensen, Solvejg
Gas phase nitration and oxidation of cresol initiated by OH or NO_3 radicals in presence of NO_2
- PI-012. Uhe, Andreas
Application of the energetic span model to catalyst development – Coupling of CO_2 and arene C-H bonds
- PI-013. Magalhães, Alexandre
DFT study of metallosalen complexes as the basis of metal cation sensors
- PI-014. Lain, Luis
Applications of the effectively unpaired electron density matrix to the study of electronic correlation
- PI-015. Torre, Alicia
Studies of local spin in Hilbert and three-dimensional physical spaces
- PI-016. Ishida, Toshimasa
Non-adiabatic ab initio dynamics of 11-cis retinal photoisomerization
- PI-017. Sastre, German
Transition Metal $\cdots H_2$ interactions in Metal-Organic Frameworks
- PI-018. Ivanov, Petko
Macrorings and complex molecular systems with potential useful applications
- PI-019. Yadava, Umesh
Gas Phase Conformational Studies on Some Pyrazolo[3,4-d]pyrimidine derivatives
- PI-020. Bulusheva, Lyubov
Quantum-chemical modelling of CdS specie formation on the graphitic surface
- PI-021. Archirel, Pierre
UV-visible absorption spectra of platinum carbonyl complexes and particles
- PI-022. Yoshida, Norio
Electronic structure theory of biomolecules in solution
- PI-023. Furuhamo, Ayako
A reaction between alpha beta unsaturated carbonyl chemical substance, a water molecule, and thiol moiety in biomolecule: aiming to eco-toxicity prediction

- PI-024. Li, Xin
Primary Events of Photodynamics of GFP Chromophores in Different Environments
- PI-025. Barbatti, Mario
Urocanic acid unveiled – anomalous photophysics caused by tautomeric effects
- PI-026. Crespo Otero, Rachel
Cr(CO)₆ photochemistry: UV absorption spectral intensities and dynamics of photodissociation
- PI-027. Ørnsø, Kristian Baruël
A study of the performance of DFT calculations on the different spin multiplicities of iron(III)mono-oxide
- PI-028. Martínez, Lara
On the population of triplet states in 6-thioguanine: first steps towards the generation of singlet oxygen
- PI-029. Saad Saoud, Fatma
Mechanism of the phase transition in GaN under pressure up to 100 GPa
- PI-030. Armangué Fraixinó, Lluís
NMR chemical shifts in nucleotides: influence of the Mg (II) coordination site
- PI-031. Gámez, José A.
Is the Se-Se bond cleavage the most favourable process in the electron attachment to diselenides? The importance of asymmetry
- PI-032. (Previous PIII-063) Ivanova, Nina
Intermolecular interaction energy in complexes of copper and iron sulfodes with vinyl acetylenic alcohols
- PI-033. Sicilia, Emilia
Theoretical investigation of the mechanistic aspects of homogeneous processes for hydrogen storage
- PI-034. Rimola, Albert
Interstellar glycine formation occurring at surfaces of ice water dust grain particles under ionizing effects
- PI-035. Goerigk, Lars
Which density functionals can be reliably applied to main group thermochemistry?
- PI-036. Deleuze, Michael S.
Many-Body calculations of electric polarizabilities in asymptotically complete basis sets
- PI-037. Ponec, Robert
Bonding quandary in Cu₃S₂ core. Insights from the analysis of domain averaged Fermi holes and the analysis of the local spin
- PI-038. Marzouk, Asma
Non-dynamical correlation in the Cobalt+O₂ interaction: a challenge for the new meta-GGA functionals
- PI-039. Tuvi-Arad, Inbal
Asymmetry, asynchronicity and reactivity of a symmetrically substituted cycloaddition reaction
- PI-040. Bahri, Hajer
Primary and secondary kinetic isotope effects on the gas phase reactions H₂O₂+X (X=H, Cl)
- PI-041. Olsen, Jógvan Magnus
Molecular properties through polarizable embedding
- PI-042. Derbel, Najoua
Theoretical study of guanidino-phenol based antibacterial compounds
- PI-043. Provorse, Makenzie
Distinguishing features between proton-coupled electron transfer and hydrogen atom transfer from multistate DFT
- PI-044. Bischoff, Florian A.
Low-order tensor approximations for electronic wave functions: Hartree-Fock method with guaranteed precision
- PI-045. Baglayan, Özge
DFT study of solvent effects on conformational equilibria and vibrational spectra of 1-cyclobutylpiperazine
- PI-046 (previous PIII-072) Gökcan, Hatice
Theoretical modeling of GABA degradation and inactivation mechanism of GABA-AT
- PI-047. Kurita, Noriyuki
A combined green's function and density-functional study of electrical conductivity of artificial DNA duplexes

- PI-048. Rosi, Marzio
Theoretical study of reactions relevant for atmospheric models of Titan: excited nitrogen atoms with CH₄, C₂H₄ and C₂H₆
- PI-049. Pichugina, Daria
Application of quantum-chemical methods for gold nanoparticles study
- PI-050. Zhao, Junfang
Structures of a₄⁺ and a₄⁰ fragments derived from protonated pentaglycine: density functional theory calculations and IRMPD spectroscopy
- PI-051. Liao, Hsin-Yi
Computational study of the substitution effect on the mechanism for the gold(I)-catalyzed ring expansions of unactivated alkynylcyclopropanes
- PI-052. Sakai, Shogo
Structures Prediction and Aromaticity for Condensed Polycyclic Hydrocarbons
- PI-053. Zhanpeisov, Nurbosyn U.
Theoretical DFT study on structure and chemical activity of transition metal oxides, carbon K4 and metal-organic framework IRMOF structures
- PI-054. Simón, Luis
How reliable are DFT transition structures?
- PI-055. Karton, Amir
Mechanistic investigation of the high reactivity and specificity of peroxiredoxins with peroxides
- PI-056. Mallick, Dibyendu
Selectivity of Bispropargyl Sulfone under Basic Conditions: A Theoretical and Experimental Study
- PI-057. Geldof, Davy
An extension of the Hirshfeld method to open shell systems using fractional occupations
- PI-058. Vargas-Fuentes, Crisa
A density functional theory study of the 'mythic' Lindlar hydrogenation catalyst
- PI-059. Monge-Palacios, Manuel
Dynamics study of the Cl(²P) + NH₃ reaction with QCT calculations. Influence of the reactant well
- PI-060. Milhøj, Birgitte Olai
On the use of Local Dense Basis Sets in the Calculation of EPR Hyperfine Couplings. A study on a Model System for Cytochrome P450
- PI-061. Saenz Méndez, Patricia
Insights into the structural basis of microtubule stabilizing antitumoral agents (MSAAs) activity. Prediction of the binding modes of Taxol and Laulimalide
- PI-062. Lin, Jyh Shing
DFT-based molecular dynamics study of self-coupling reaction of CH₃-C≡C_(ads) adsorbed on Ag(111) surface
- PI-063. Patil, Mahendra
A QM/MM approach to excited-state dynamics of light harvesting peridinin-chlorophyll-a protein (PCP) complexes
- PI-064. Verzeni, Riccardo
CASSCF/CASPT2 studies of the photophysics of dithiosubstituted formic acid dimers
- PI-065. Díaz, Cristina
Self-assembly of TCNQ on Cu(111)
- PI-066. Tafipolskiy, Maxim
Accurate Force Fields from First Principles: New Trends
- PI-067. Perrier, Aurelie
Photoinduced Intramolecular Charge Transfer Process of pyridinium betaine: a theoretical spectroscopic study
- PI-068. Uhl, Elmar
Theoretical study of d→s electronic transitions in NaF:Cu⁺ lattices allowed by vibronic coupling
- PI-069. Yoshioka, Yasunori
Theoretical Study on Intermediates from S₀ to S₁ States of OEC in Photosystem II
- PI-070. Mitani, Masaki
A B3LYP study on hydration of K⁺ and Na⁺ ions in the cavity of the KcsA potassium channel

- PI-071. Chan, Bun
G4(MP2)-6X: pay for G4(MP2) and get G4 performance
- PI-072. Shojaei, Seyed Hamid Reza
Electron momentum spectroscopy of pyrimidine at the benchmark ADC(3) level
- PI-073. Motta, Alessandro
Adsorption at the solid-liquid interface with ab initio MD: the case of glycine on boehmite
- PI-074. Piris, Mario
Theoretical Foundations of PNOF
- PI-075. Fdez. Galván, Ignacio
Solvent effects on the dual fluorescence of 1-phenylpyrrole
- PI-076. Jiménez-Izal, Elisa
Designed porous solids based on endohedrally doped CdS nanoclusters
- PI-077. Ribas Ariño, Jordi
Rationalizing the stereoselectivity of proline-catalyzed asymmetric aldol reactions in water
- PI-078. Nova, Ainara
Mechanistic study of the carboxylation of aryl bromides with CO₂
- PI-079. Weymuth, Thomas
Can Raman optical activity discriminate between different types of protein β -turns?
- PI-080. Haag, Moritz
Automatic generation and refinement of potential energy surfaces using IMLS fits of different order
- PI-081. Bessac, Fabienne
Pesticide interaction with environmentally important cations: a theoretical study of atrazine
- PI-082. Ito, Mika
Mechanistic insights into effects of ligands on unfolding of the amyloid β -peptide central helix
- PI-083. Finkelmann, Arndt
Oxygen coordination to the active site of Hmd in relation to [FeFe] hydrogenase
- PI-084. Cembran, Alessandro
Block-Localized Wavefunction: A Powerful Tool To Investigate Intermolecular Interactions
- PI-085. Steenbergen, Krista G.
Modelling the superheating of small gallium and aluminium clusters
- PI-086. Fortenberry, Ryan
Theoretical Prediction of New Dipole-Bound Singlet States for Anions of Interstellar Interest
- PI-087. Chen, Hsing-Yu
Variation in electronic transport of semiconducting single-walled carbon nanotubes due to NO₂ adsorption
- PI-088. (Previous PIII-088) Al-Hashimi, Nessreen
A comparison of a hybrid functional; DFT versus ab-initio calculations in the reaction of iodine with n-electron donors
- PI-089. Schmidt, Sebastian
Rh-catalyzed hydroformylation of butadiene: a systematic screening of intermediates and reaction pathways using DFT and DFT-D
- PI-090. Boguslawski, Katharina
CASCI-Type wave function expansions for very large active spaces
- PI-091. Hakkim, V
Catalytic mechanism of cobalt carbonic anhydrase: a density functional theory (DFT) investigation
- PI-092. Broeckaert, Lies
DFT study of the electroreduction of aromatic esters
- PI-093. Rajapandian, V
A systematic study on the force field parameters for the copper proteins
- PI-094. Trummel, Aleksander
Calculation of pK_a of superacids in 1,2-dichloroethane
- PI-095. Sato, Kanako
Geometries and Electronic Structures of Hg_n Clusters (n=1-10)

- PI-096. Escudero Masa, Daniel
RASPT2 vs long-range/hybrid TDDFT methods: benchmarking the excited states of Ru(II) polypyridyl complexes
- PI-097. Wu, Min
Theoretical study of pyridoxine (vitamin B6) photolysis
- PI-098. Ruiperez, Fernando
Electronic structure and bonding in heteronuclear transition metal dimers. A CASSCF/CASPT2 study
- PI-099. Tian, Boxue
Catalytic mechanism of an unusual flavoprotein monooxygenase, 2-methyl-3-hydroxypyridine-5-carboxylic acid oxygenase: an ONIOM/DFT study
- PI-100. Quiñero, David
Study of anion- π interactions and cooperativity effects in RNA-protein binding
- PI-101. Garcia-Borràs, Marc
Exploring the exohedral reactivity of the titanium carbide endohedral metallofullerene: $Ti_2C_2@D_{3h}-C_{78}$
- PI-102. Fernández García-Prieto, Francisco
Solvent effects on the absorption spectra and conformational equilibrium in the p-coumaric acid and derivatives
- PI-103. Lupan, Alexandru
Performance of the computational methods for modeling alpha helical structures
- PI-104. García, Gregorio J.
Thiophene-based discotic systems as precursors of organic semiconductors: A DFT study
- PI-105. Hirayama, Natsumi
Hydrolysis of anticancer platinum complexes: a relativistic FMO-MD study
- PI-106. Johansson, Mikael
Modelling the polymerisation mechanism of α -diimine iron catalysts
- PI-107. Naruse, Yuji
Geminal Bond Participation in Carroll Rearrangement
- PI-108. Krauter, Caroline M.
Photophysics of coumarin and its hydroxysubstituted derivatives
- PI-109. Faßhauer, Elke
Relativistic lifetimes of innervalent ionized states
- PI-110. El Hamdi, Majid
On the relative stability of the XAAX and X_2A_2 isomers ($X = H, F, Cl, Br, I, Li, Na; A = S, O$)
- PI-111. Gopakumar, G
Theoretical studies on the mechanism and stereoselectivity of palladium catalyzed allylic alkylation
- PI-112. Altarsha, Muhannad
 β -Cyclodextrins in Supercritical CO_2 : a Molecular Dynamics Study
- PI-113. Moral Muñoz, Mónica
DFT study of poly(aril-s-tetrazines) as n-type conducting materials
- PI-114. Marin, Ray
Efficient use of accessibility in microRNA target prediction
- PI-115. Larrañaga Agirre, Olatz
Elucidation of the key steps of the mechanism of the Morita-Baylis-Hillman reaction: the role of the Lewis bases and protic additives
- PI-116. Aravena, Daniel
Magnetism and quantum transport in Cr_7Ni complexes
- PI-117. Wang, Yang
Catalytic role of surface in the anti-syn isomerization of DCNQI at Cu(100) substrate
- PI-118. De Cózar Ruano, Abel
Computational kinetics of the reaction between cyclic anhydrides and imines
- PI-119. Martín, Fernando
On the shell effect of $(C_{60}-He_n)^+$ complexes in helium droplets

- PI-120. Morales, Noelia
A Comparative Molecular Dynamics Study: Lanthanides (III) vs Actinides (III)
- PI-121. Rayón, Victor M
Benchmark calculations on monoligand complexes of Ca and Mg: assessment of molecular mechanics potentials
- PI-122. Hamidi, Mohamed
Theoretical study of Donor-Acceptor copolymers based on thiadiazolothienopyrazine for photovoltaic device applications
- PI-123. Gómez, Hansel
Computational study of glycosyltransferases mechanisms
- PI-124. Pérez, Andrea
Octahedral complexes of the series of actinides hexafluorides
- PI-125. Laczowski, Krzysztof
Optically induced birefringences in model systems. An ab initio and density functional study
- PI-126. Kim, Seonah
Computational design of enzymes for the aromatic Claisen rearrangement
- PI-127. Fan, Kang-Nian
A theoretical study on the deep oxidation in the ODH reaction of propane over V₂O₅ (001) surface
- PI-128. Frontera, Antonio
On the directionality of anion- π interactions
- PI-129. Schebarchov, Dmitri
Investigating the electronic structure and polymorphism of gallium clusters
- PI-130. Lavín, Carmen
Oscillator strengths and emission branching ratios for lines of the $c_4'1\Sigma_u^+(3)-X^1\Sigma_g^+(0-5)$ bands of N₂
- PI-131. Keltner, Anne-Marie
Solvent effect on the photophysics of 7-substituted 3,4-dicyano-6-methoxy-carbostyryl: TDA versus TD-DFT
- PI-132. Senthilnathan, Dhurairajan
Bio-inspired materials for H₂ production and oxidation: multiscale mechanistic modeling of the electrocatalytic processes on [Ni (PNP)₂]²⁺ complexes
- PI-133. Higashi, Masahiro
Direct simulation of excited-state intramolecular proton transfer of 10-hydroxybenzo[h]quinoline in solution
- PI-135. (Previous PIII-102) Christian, Gemma J.
Theoretically Probing the Nature of Superoxide Species in Extradiol Enzymes
- PI-136. Steinmetz, Marc
Performance of the new double hybrid PWPB95 for organic activation reactions with Pd and Ni
- PI-137. Schirmer, Birgitta
Activation of Conjugated-Ynones with Frustrated Lewis Pairs – Metal-Free Hydrogenation of the C-C Triple Bond
- PI-138. Lakuntza, Oier
Methane activation by HNiOH⁺
- PI-139. Kruse, Holger
Theoretical investigation of nucleobase quadruplex interactions in G-DNA model systems
- PI-140. Rodríguez, A. M.
Why does microwave improve cyclotrimerization reactions? A DFT study
- PI-141. Risthaus, Tobias
Investigation of the mixing gap in fluoroalkane - alkane systems by DFT and MC methods
- PI-142. Zhang, Xueqing
Modelling the Initial Stage of Zeolite Synthesis
- PI-143. Allison, Jane
Local elevation biasing: a novel method for generating ensembles of structures that fit experimental data
- PI-144. Kwiecien, Renata Anna
Nicotine degradation: effect of geometry on alternative reaction pathways
- PI-145. Heidenreich, Andreas
Laser pulse length dependence of electron and nuclear dynamics in Coulomb explosions of xenon clusters

- PI-146. Donald, Steven
Nitrogen fixation to produce ammonia: finding the ideal catalyst system via computational screening methods
- PI-147. Nava, Paola
Computational studies on carbon-carbon bond activation by transition metals
- PI-148. Liao, Rong-Zhen
Comparison of QM-only and QM/MM Models for the Mechanism of Tungsten-Dependent Acetylene Hydratase
- PI-149. Katz, Aline
Determination of bromide and iodide ions parameters for use in molecular simulations of TIP3P compatible solvated systems with CHARMM27 force field.
- PI-150. Heggen, Berit
Nonadiabatic Decay Dynamics of Purine Nucleobases in Aqueous Solution
- PI-151. Plata, José Javier
Electronic properties and structure of 1d ceria materials: from atomistic to nanoscale models
- PI-152. Stradi, Daniele
Effect of dispersion interactions on the structure of graphene monolayer over Ru(0001)
- PI-153. Danovich, David
No-pair bonding in the highest spin states of mixed copper-gold metal clusters based on ab initio, DFT and valence bond analysis
- PI-154. (Previous PIII-183) Soares, Ricardo
Characterization of the standalone stability of domain III of dengue virus "E" protein
- PI-155. Sánchez-Sanz, Goar
Chiral discrimination in compounds with chalcogen-chalcogen interactions
- PI-156. Rocha, Alexandre
Core hole localization in N₂: an old problem, a new solution
- PI-157. Zhu, Chaoyuan
Analytical formula of anharmonic Franck-Condon factors and its application to molecular electronic spectroscopy
- PI-158. Lundell, Jan
Vibrational spectroscopy of HXeSH and HXeSH...H₂S
- PI-159. Weinberg, Josette
Theoretical study of 5-HTP. Potential new drug resulting from the complexation of 5-HTP with ATP
- PI-160. Olbert-Majkut, Adriana
Raman spectroscopy of small hydrogen-bonded carboxylic acid complexes
- PI-161. Ali-Torres, Jorge
Structures and stabilities of Fe^{2+/3+} complexes relevant to Alzheimer's disease: an ab initio study
- PI-162. La Porta, Felipe
First principles calculations on the photoluminescence behaviour of BaZrO₃ nanocrystals
- PI-163. Day, Paul
Modeling reactivity of aluminum nanocluster anions with water for hydrogen production
- PI-164. Borštnar, Rok
Irreversible Inhibition of Monoamine Oxidase B: A Computational Study
- PI-165. Le, Hai Anh
Towards an accurate and efficient computation of interaction energies between flexible proteins
- PI-166. Bettens, Ryan P. A.
An alternative energy based molecular fragmentation algorithm
- PI-167. Suárez, Dimas
A computational model for triple helical peptide binding to the catalytic domain of matrix metalloproteinases
- PI-168. Petrauskas, Vytautas
Empirical model of macromolecule-ligand interaction
- PI-169. Kabelác, Martin
Structure and conformational behavior of the DNA oligonucleotide attached to the charged surface: A Molecular Dynamics Study

- PI-170. Liu, Ya-Ling
Identification of anti-inflammatory compounds in Anrodia camphorate through docking simulation onto glucocorticoid receptor
- PI-171. Luis, Josep Maria
Fine-tunable metalloporphyrinic nanocapsules as hosts for fullerenes
- PI-172. Muñoz, Francisco
DFT study on phospholipids mediated decomposition on hydrogen peroxide
- PI-173 (Previous PIII-254) Engel, Hamutal
Nuclear quantum effects in enzyme catalysis – From development to application
- PI-174. Gao, Chunxia
Simulation studies of protein-protein interaction between K-Ras and P120GAP
- PI-175. Kristyan, Sandor
Statistical analysis of the electron-electron repulsion energy term in Hartree-Fock SCF calculation in view of algebraic expression, rotation, vibration and convergence of the LCAO parameters. Application and test with phospholipids.
- PI-176. Dobado, José A.
CoNTub 2.0: A three-nanotube junction model constructor
- PI-178. Azpiroz, Jon M.
Interaction between Zn₆S₆ nanocluster and organic ligands
- PI-179. Petkovic, Milena
O-H Stretching dynamics in phenol and its hydrogen bonded complexes
- PI-180. Pershina, Valeria
Is element 114 a noble gas or a metal? The answer from the relativistic quantum theory
- PI-181. Sikk, Lauri
Computational study of copper-free Sonogashira cross-coupling reaction
- PI-182. Nadal-Ferret, Marc
A method to compute probability current in generic coordinates: an application to the tunneling contribution in green fluorescent protein
- PI-183. Parasuk, Waraporn
Stereoselectivity of Strecker reaction catalyzed by titanium-N-salicylyl-β-aminoalcohol complex: a DFT study
- PI-184. Parasuk, Vudhichai
What is the Coordination Number of Copper-water Complex?
- PI-185. Daru, Janos
Theoretical Study on the Mechanism of the von Pechmann reaction
- PI-186. Lee, Wook
Theoretical elucidation of the protonation states of the catalytic residues in mtKasA
- PI-188. Redondo, Pilar
Comparative kinetical study of the C-H bond activation in methyl fluoride by third-row cations in gas phase
- PI-189. Adamson, Aiko
Computational study of N-substituted amine-borane complexes
- PI-190. Curutchet, Carles
Triplet-triplet energy transfer in DNA: a process that occurs on the nanosecond timescale
- PI-191. Filhol, Jean-Sébastien
Ab initio electrochemistry at the interface of materials
- PI-193. Izsak, Robert
An Overlap Fitted RIJCOSX Theory
- PI-194. Szatylowicz, Halina
H-bonded complexes of formamide: the influence of computational level on quality of results
- PI-195. Marchal, Rémi
On the understanding of the architectures of small ligated aluminium clusters
- PI-196. Lesar, Antonija
Mechanism of the radical reaction of CH₃SO with NO₂: DFT and ab initio studies

- PI-197. Aparicio-Anglès, Xavier
Adsorption of $\text{SiW}_{12}\text{O}_{40}^{4-}$ on silver surface: immediate reduction of the polyoxometalate
- PI-198. Fajín, José Luis C.
A DFT study of the NO reduction by CO on gold based catalysts
- PI-199. Chermette, Henry
Fragmentation Mechanism of DNA bases
- PI-200. Ortega-Carrasco, Elisabeth
Computational study of the activation process of an artificial metalloenzyme
- PI-201. Mollenhauer, Doreen
Theoretical study of pyridine derivatives in interaction with gold nanoparticles
- PI-202. Solans-Monfort, Xavier
Mechanistic insights into the activation of grubbs-hoveyda olefin metathesis precatalysts: the key role of the olefin coordination and decoordination steps
- PI-203. Horbatenko, Yevhen
 $\text{Si}\cdots\text{H}\cdots\text{Si}$ interligand interactions in organometallic complexes
- PI-204. Caricato, Marco
Excited states in solution at EOM-CCSD level with the polarizable continuum model of solvation
- PI-205. Richardson, Jeremy
Ring-polymer instanton method for calculating rates and tunnelling splittings
- PI-206. Barrientos, Carmen
Neutral polycyanides of transition metals
- PI-207. Nuñez-Zarur, Francisco
Effects of reactant substituents on the ring closing 1,6-enyne metathesis reaction: origin of the exo/endo selectivity with Ru-based catalysts
- PI-208. Mandado, Marcos
Definition of exchange and correlation densities using natural orbital CI expansions
- PI-209. Chipman, Daniel
Modeling short-range contributions to hydration energies
- PI-210. Wedig, Ulrich
Relativistic effects on homonuclear triel clusters
- PI-212. Mollica, Cesare
Dephasing representation: defeating the efficiency of both quantum and classical simulations with semiclassics
- PI-213. Roskop, Luke
Implementation of quasi-degenerate second-order perturbation theory for ORMAS-SCF reference functions
- PI-214. Lamsabhi, Al Mokhtar
Tautomerism in Uracil: A different View
- PI-215. Vyboishchikov, Sergei
Molecules with multiple $\text{Si}\cdots\text{H}$ interactions: structure and dynamics
- PI-216. Drici, Nedjouda
Insight into structural properties of NCp7 proximal zinc finger: long-range electrostatic interactions effect on molecular dynamic simulations.
- PI-217. Alvarez-Thon, Luis
The effect of the spin-orbit interaction on the ground state of RhF_6 and IrF_6 complexes
- PI-218. Head, John
DFT Investigation of the Organic Desulfurization Ability by Mo_3S_x ($x = 0-12$) Nanoclusters
- PI-219. Zhang, Peng
Dipole preserving and polarization consistent charges
- PI-220. Eizaguirre, Ane
Theoretical and experimental study of formamide- Sr^{2+} reactions in the gas phase
- PI-221. Nguyen, Kiet
The Long-range-corrected Methods for DFT Hybrid Functionals

- PI-223. Díaz, Natalia
A computational study of the triple helical peptide binding to the full-length MMP-2 enzyme
- PI-224. Ohno, Koichi
Automated Web-Browser Visualization of the Whole Lists of Chemical Structures and Reaction Channels Explored by the Global Reaction Route Mapping Method
- PI-225. Mieda, Shunsuke
Theoretical study on differences between dipole moments of L-amino acid residues and D-amino acid residues
- PI-226. Madzhidov, Timur
Electronic structure of organoselenium compounds and their complexes with electron acceptors of different types
- PI-227. Sánchez, Juan Pablo
High level calculations on $C_{54}H_{18}/H_2$: A simple model of the adsorption of hydrogen on graphene
- PI-228. Arabi, Alya
The Assessment of a Nonempirical DFT Functional for van der Waals Complexes at Nonequilibrium Geometries
- PI-229. De Vleeschouwer, Freija
Design of substituted naphthols with optimal acidity and photoacidity
- PI-230. Uta, Matei-Maria
The Sphericity of the Diverse Ten-Vertex Polyhedra Found in Post-Transition Metal Clusters: Germanium Clusters with Interstitial Magnesium Atoms as Model Systems
- PI-231. Pérez-Juste, Ignacio
Enhanced Raman Scattering of Pyridine Adsorbed on a Carbon Surface
- PI-232. Yu, Jen-Shiang K.
Theoretical study of the Rydberg states of xenon and radon dimers
- PI-233. Lein, Matthias
The interplay of theory and experiment for highly fluxional compounds. Structural determination through computed NMR spectra
- PI-234. Hurtado, Marcela
Gas-phase acidity of oxygen, sulfur, selenium and tellurium cyclopentadienyl derivatives
- PI-235. De Proft, Frank
Design of molecules with optimal density functional theory reactivity indices
- PI-236. Christensen, Anders Steen
Inferential protein structure determination and refinement using backbone chemical shifts
- PI-237. Anoop, Anakuthil
Computational study of the enzymatic oxetane formation in the biosynthesis of Taxol
- PI-238. De Lima, Guilherme
Water Adsorption on the Reconstructed (001) Chalcopyrite Surface
- PI-240. Irgibaeva, Irina
DFT(SLYP) calculation of intermediates of α -, β -hydroxyethyl radicals electroreduction
- PI-241. Sliwa, Pawel
DFT study of hydroxyacetylene polymerization catalysed by ruthenium complexes
- PI-242. Wilson, David
Molecular properties of ferrocene
- PI-243. Aldongarov, Anuar
Calculation of spectral-luminescent properties of polymer composition of polyvinyl alcohol and rhodamine B
- PI-244. Bankiewicz, Barbara
QTAIM parameters in H-bond critical point vs. Interaction energy components (SAPT) – the case of charge assisted hydrogen bonding
- PI-245. Chmurzynski, Lech
Theoretical studies on association in substituted phenol anionic systems in acetonitrile using potential of mean force
- PI-246. Saitow, Masaaki
Excitation propagator approach augmented with self-energy shifting
- PI-247. Aquino, Adelia
Interactions of organic compounds with soil components – elucidating mechanisms on a molecular level

- PI-248. Vummaleti, S. V. Chaitanya
Theoretical insights into the mechanism of carbon monoxide (CO) liberation from co-releasing molecules: a DFT study
- PI-250. Courcot, Blandine
Computational strategies for molecular mechanics force field optimizations
- PI-251. Isegawa, Miho
Incorporation of charge transfer into the explicit polarization (X-Pol) potential by grand canonical DFT
- PI-252. Kudo, Takako
Ab initio MO and DFT Study for the isomerization of Bicyclo[1.1.0]tetrasilane and the germanium analogues
- PI-253. Deng, Chunmei
Theoretical prediction on fluorescence quantum efficiency of pyrazine derivatives: an explanation for aggregation induced emission
- PI-254. Fujiwara, Takayuki
FMO-MD simulations for hydrated trivalent lanthanide ions
- PI-255. Giorgi, Giacomo
Precursor optical excitations of photocatalysis at the (001) surface of TiO₂ anatase
- PI-256. Maciel, Cleiton
Molecular dynamics study of C₆₀ solvation in ionic liquids
- PI-258. Jongkon, Nipa
A possible mechanism of sialidase (neuraminidase): quantum calculation approaches
- PI-259. Liang, Xiao
Local Site Selectivity, Conformational Structures and Free Energy Landscapes of Acid Catalysed Hydrolysis of Ether Bonds in Aqueous Solution
- PI-260. Montoya, Alejandro
Thermodynamic analysis of ammonia oxidation on Co₃O₄
- PI-261. Somboon, Tuanjai
DFT studies on arabidopsis thaliana allene oxide synthase
- PI-262. Osuna, Silvia
Dispersion corrections are essential for the study of chemical reactivity in fullerenes
- PI-263. Wells, Brad
Simulation of gas adsorption in model zeolitic imidazole frameworks for the capture of CO₂
- PI-264. Park, Seung
Reaction dynamics of O(³P) + C₃H₃ on a full dimensional potential energy surface
- PI-265. Sharma, Akhilesh Kumar
In search of active species in proline catalyzed asymmetric organocatalytic reactions
- PI-266. Shailendra, Asthana
Inactivation of BVDV RdRp upon mutation I261M: an explanation from computer simulations
- PI-267. Hirano, Toshiyuki
ProteinDF: high performance all-electron canonical calculation program for proteins
- PI-268. Shiga, Motoyuki
Ab initio path integral simulations of hydrogen bonded systems
- PI-269. Ghysels, An
Monte Carlo simulations to understand "breathing" phenomenon of Metal Organic Frameworks
- PI-270. Friese, Daniel H.
Fast correlated second-order property calculations: 2nd derivatives for RI-CC2 and RI-MP2
- PI-271. Fogarasi, Geza
Intramolecular Proton Transfer in Biomolecules as Investigated by Quantum Chemistry and Molecular Dynamics
- PI-272. Hediger, Martin
Towards the introduction of amidase activity in Candida Antarctica Lipase B (CaLB)
- PI-273. Zanti, Giuseppe
Theoretical investigation of bimetallic palladium-gold clusters (Pd_nAu_m)

- PI-274. Walter, Christof
Investigation of a Five-Membered-Ring Allene and Related Model Systems
- PI-275. Zacarias, Angelica
3D orientation of the transition dipole moment of chlorophyll, coumarine and corrole: A study combining UV-pump IR-probe spectroscopy and DFT calculations
- PI-276. Gritsan, Nina P.
Reactivity of Thiophenolate toward chalcogenadiazoles
- PI-277. Kamisaka, Hideyuki
Theoretical Comparison of Structural Stability between Two Polymorphs: Defective Nb-doped Anatase and Rutile TiO₂
- PI-278. Kozlov, Sergey
CH_xO and CH_x species (X = 1-3) on a palladium nanoparticle representing model catalysts
- PI-279. Freitas, Gabriel
The role of the interference effect in earth-alkaline compounds
- PI-280. Sen, Kakali
Investigation of molecular oxygen activation in P450eryF using hybrid QM/MM methodology
- PI-281. Von Hopffgarten, Moritz
The Maximum Coordination Number in [M(EH)_n] Compounds (E = Zn, Cd, Hg)
- PI-282. Korth, Martin
Third-generation Hydrogen-bonding Corrections For Semiempirical QM Methods and Force Fields
- PI-283. Hölscher, Markus
Challenges in the computational investigation of Rhodium pincer complex catalyzed hydroamination of C₂H₄ with NH₃

POSTER SESSION II - (PII-1 to PII-299)
Tuesday, July 19 - 11.30-13.30h (Faculty of Economy)

- PII-001. Gekas, George
Thallium(I) "full" Pt_3TIpt_3 and "open-face" $TIpt_3$ sandwich versus their "naked" $Pt_3(\mu_2-L)_3(L')_3$ triangular units: A DFT study of their bonding, photophysical properties and possible application in OLED devices
- PII-002. Escribano, Rafael
Proton transfer and autoionization in $HNO_3.HCl.(H_2O)_n$ particles
- PII-003. Shang, Yuan
Theoretical study of the influences of electron-hole pair dissociation and decay rates on the polymer photovoltaic performance
- PII-004. Ben Fredj, Arij
Importance of water molecules on the stability of the chlorophyll-a dimer
- PII-005. Gonthier, Jérôme
Four-electron reduction of O_2 by tetrathiafulvalene
- PII-006. Vijay Solomon, Rajadurai
Can computational mutagenesis provide clues to develop better breast cancer drugs?
- PII-007. Jaccob, Madhavan
Computational modeling of mechanistic aspects of transition metal mediated catalytic reactions
- PII-008. Elroby, Shabaan
Theoretical investigation to understand the photochemical reaction mechanism of decarbonylation of cyclopropanone
- PII-009. Vilaseca, Eudald
Diffusion in macromolecular crowded media: Monte Carlo simulation of obstructed diffusion vs. FRAP experiments
- PII-010. Stradomska, Anna
Vibronic coupling of charge-transfer excitons in the sexithiophene crystal
- PII-011. Markovic, Marijana
Can MD simulations of solvated bis(L-isoleucinato)copper(II) in aqueous solution explain a disorder in the x-ray crystal structure
- PII-012. Steiner, Denise
Calculation of binding free energies of inhibitors to plasmepsin II
- PII-013. Cheron, Nicolas
The mechanism of the Ugi reactions
- PII-014. Álvarez-Barcia, Sonia
The oxidation of Al atoms embedded in water clusters
- PII-015. Grabar, Marina
Molecular modeling of new permanently charged phenanthridinium-nucleobase conjugates in complexes with double stranded polynucleotides
- PII-016. Bertoša, Branimir
Investigation of anticancer activity of heterocyclic amides and quinolones using 3D-QSAR analysis
- PII-017. Jin, Bih-Yaw
Quantum Transport Through a Simple Electron-Phonon System with Electron Correlation
- PII-018. Budzak, Simon
Benchmark study of charge transfer excitation in methyl substituted benzene and tetracyanoethylene complexes
- PII-019. Ohanessian, Gilles
Structures and Vibrational spectra of sodiated peptides
- PII-020. Tussupbayev, Samat
Mechanism of ammonia formation by metal-ligand cooperative hydrogenolysis of a nitrido complex
- PII-021. Vega, M^a Victoria
Calculations of the photoionization cross sections and asymmetry parameters in molecules
- PII-022. Medved, Miroslav
NLO Responses of π -conjugated oligomers containing carbon, boron and nitrogen skeleton atoms

- PII-023. Muñoz-Losa, Aurora
Solvent effects on the radiative and nonradiative decay of a model of the rhodopsin chromophore
- PII-024. Poblador-Bahamonde, Amalia
Importance of the relativistic effects for reproducing the experimental ^{29}Si NMR shifts for a series of $\text{RuCp}(\text{PMe}_3)_2(\text{SiX}_3)$ complexes
- PII-025. Tsou, Chia-Chin
Electronic Structures and Structural Instabilities in Infinite Extended Metal Atom Chains
- PII-026. Pavošević, Fabijan
Bond-stretch isomerism in 1,3-disilabicyclo[1.1.0]butane by the computational chemistry approach
- PII-027. Yeguas, Violeta
 β -Cyclodextrin-peptide inclusion complexes: Insights from theory
- PII-028. Gil, Adrià
A journey to the centre of polyoxoperoxouranates. Close encounters between theory and experiment
- PII-029. Borosky, Gabriela
Computational study related to the mutagenic activity of heterocyclic aromatic amines
- PII-030. Karlicky, Frantisek
Graphene fluoride – the thinnest insulator and a route to graphene-based semiconductors
- PII-031. Krejčíková, Simona
Doped titania photocatalysts for polluted water cleaning; preparation and characterization
- PII-032. Maletrova, Ywetta
Comparison of various titania photocatalysts by the contaminated water cleaning
- PII-033. Mach, Taylor J.
Gauge-invariant coupled cluster response theory for chiroptical properties
- PII-034. Nedyalkova, Miroslava
Ion distribution around charged spherical colloids from molecular dynamics calculations with explicit water molecules
- PII-035. Solcova, Olga
Thorough characterization of prepared TiO_2 - ZrO_2 mixed oxides for photocatalytic oxidation
- PII-036. Sanz, Pablo
A methodology for parallelizing a legacy AIM sequential code on multicore computing systems
- PII-037. Senn, Florian
Investigations of $[\text{GdDOTA}(\text{H}_2\text{O})]^-$ Zero Field Splitting
- PII-038. Hankova, Libuse
Modeling of swollen state morphology of functional polymers
- PII-039. Matito, Eduard
Performance of density functional methods on the two lowest-lying states of three-electron harmonium atom
- PII-040. Rashid, Zahid
Resonance and aromaticity of polycyclic conjugated hydrocarbons: an ab initio valence bond approach
- PII-041. Nguyen, Thi Ai Nhung
Bonding situation in $(\text{CO})_5\text{W-E}(\text{PPh}_3)_2$ complexes with $\text{E}=\text{C}-\text{Pb}$
- PII-042. Devarajan, Deepa
Are they linear, bent or cyclic? Quantum chemical investigation of the heavier analogues of HCN-HNC
- PII-043 (Previous PI-032) Marino, Tiziana
*Arylsulfatase enzyme from *Pseudomonas aeruginosa* as example of promiscuous enzyme: a theoretical point of view*
- PII-044. Ruiz-Pernía, José Javier
Beyond the distinguished reaction coordinate. A new collective coordinate for the study of reactions in condensed phases
- PII-045. Han, Jaebeom
Balancing Polarization in the Development of an Explicit Polarization (X-Pol) Model for Water
- PII-046. Novell-Leruth, Gerard
Mechanism of HCl oxidation (Deacon process) over RuO_2

- PII-047. Almeida, João
Structure and order of hydrated lipid bilayers as studied by molecular dynamics simulation
- PII-048. Mosch, Marianne
Solvent effects on optical rotation in small chiral molecules
- PII-049. Schütt, Christian
Density functional calculations on the adsorption structures of triazatriangulenium derivatives on the Au(111) surface
- PII-050. Petit, Alban
Relative stability of 18- and 16-electron ruthenium phosphinoborane complexes : should dispersion corrections be included?
- PII-051. Berger, Robert
Analysis of vibronic transitions via time-independent cumulant expansion method
- PII-052. Berkane, Ariche
Determination of interaction parameters for Monte Carlo simulation of surfactant systems using quantum mechanical calculations
- PII-053. Fliegl, Heike
Hydrogen-bond strengths by magnetically induced currents
- PII-054. Geerke, Daan
Determination of Atomic Polarizabilities for use in Biomolecular Polarizable Force Fields
- PII-055. Segarra, Javier
Determination of the ionization potentials of water clusters (H₂O)_n [n = 2-6] by using different ab initio approaches
- PII-056. Sánchez-Marín, José
Inclusion complexes between p-curved systems: 6-CPPA@9-CPPA
- PII-057. Gusarov, Sergey
Perturbative Treatment of Exchange-Correlation Interaction obtained within the Super-CI Approach to the MCSCF Approximation
- PII-058. Aragón, Juan
Describing donor-acceptor intermolecular interactions and charge transfer excitations IN 3T-TCNQ molecular complex
- PII-059. Zapata, Felipe
Using Analytical Potential Energy Surfaces in the Dynamics of some Interesting photochemical Systems
- PII-060. Costa, Paulo
How strong can halogen bonds be? Halogen...halogen bonds in imidazolium derivatives
- PII-061. Silva, Tiago J. L.
Organometallic complexes for Non-Linear Optical Switching: DFT Evaluation of the B3LYP, CAM-B3LYP and M06 functionals
- PII-062. Da Silva, Júlio
C-H Bond Activation of Methane in Aqueous Solution: A Hybrid Quantum Mechanical/Effective Fragment Potential (QM/EFP) Study
- PII-063. Dias, Roberta
Hybrid QM/MM study of the hydroformylation reaction of propene promoted by a homogeneous Pt-Sn heterobimetallic catalyst
- PII-064. Handzlik, Jarosław
Structure of isolated Cr(VI) oxide species on silica – periodic and cluster DFT studies
- PII-065 (Previous PI-135) Calzado, Carmen J.
Polynuclear magnetic complexes: large systems, big problems
- PII-066. Lasorne, Benjamin
The electronic excited states of ethylene and large-amplitude deformations: a dynamical symmetry group investigation
- PII-067. Mondragón, Fanor
Heteroatoms effect on graphene hydrogenation
- PII-068. Tecmer, Pawel
Electronic spectroscopy of small actinide molecules: an evaluation of time-dependent density-functional theory
- PII-069. Cabral Do Couto, Paulo
Surface vs. Interior electronic excitations in water clusters: implications for QM/MM liquid water calculations

- PII-070. Bottinelli, Fiorentina
Computational study of how protonation changes affects some structural factors of dehaloperoxidase A
- PII-071. Takagi, Akira
Theoretical study of regioselectivities in the Diels-Alder reactions between substituted benzyne and furans
- PII-072. Nanbu, Shinkoh
Non-adiabatic dynamics with semiclassical trajectories: applications to photo-isomerization
- PII-073. Udvarhelyi, Anikó
Photoinduced electron transfer in a flavin-binding blue light photoreceptor
- PII-074. Escorcia, Andrés
Computational study of the O-acylation of (R,S)-propRanolol catalyzed by Candida antarctica lipase B
- PII-075. Kiselev, Vitaly
Tautomeric equilibria and thermal decomposition of nitrogen-rich heterocycles: new insights from ab initio calculations
- PII-076. Tokiwa, Hiroaki
All-Electronic Calculations (AEC)-Docking Procedure Based on the FMO-ONIOM Method
- PII-077. Andrae, Dirk
Towards a computational nanotechnology for molecular knots and links
- PII-078. Cerezo, Javier
Molecular dynamics study of the influence of oleic and 2-hydroxyoleic acids on model membranes
- PII-079. Müller, Carsten
Application of wave function based electron correlation methods to weakly bound systems
- PII-080. Grebner, Christoph
Tabu search based global optimization algorithms for problems in computational chemistry
- PII-081. Carbonniere, Philippe
The code GSAM: a global search algorithm of minima exploration for the investigation of low lying isomers of atomic and molecular clusters. Several examples from DFT-based PES.
- PII-082. Tilvez, Elkin
A DFT investigation on the acrylonitrile hydration to acrylamide catalyzed by aqueous molybdocenes
- PII-083. Degrève, Léo
The stability of extended secondary protein structures: the dengue virus E protein case.
- PII-084. Estévez, Laura
A DFT mechanistic study of neutral catalyzed condensation cure of silane modified polymers
- PII-085. Hamilton, Alexander
BINAP vs PCY₃: selective formation of different products from the same substrates
- PII-086. Otero, Nicolás
Expanding condensed Fukui functions using electron-pair density
- PII-087. Udommaneethanakit, Thanyarat
Insight into molecular interactions of Aurora-A mutants: molecular dynamics simulations
- PII-088. Heym, Peter-Paul
Virtual screening for plant PARP inhibitors to increase tolerance against abiotic stress
- PII-089. Bradshaw, Richard
Reliably and repeatably predicting free energies by combining MM-PBSA with LES
- PII-090. Giussani, Angelo
Theoretical study of the photophysics of indole by using a totally unconstrained approach
- PII-091. Ogihara, Toshihiko
A study of the phase transition temperature and bilayer structure change of phospholipid by MD method
- PII-092. Rosen, Sarah
A tough Akt to follow: understanding and predicting interactions of protein kinase B
- PII-093. Florez, Elizabeth
Effect of MgO vacancies on the reactivity of bimetallic clusters

- PII-094. Robledo, Maitreyi
Density functional theory study of exohedral metal-fullerenes
- PII-095. Rolik, Zoltán
A general-order local coupled-cluster method
- PII-096. Weng, Jingwei
Simulation of the conformational transition of the vitamin B₁₂ ABC transporter BtuCD
- PII-097. Sameera, W. M. C.
Quantum mechanics/molecular mechanics methods can be more accurate than full quantum mechanics in systems involving dispersion correlations
- PII-098. Kochumannil Varghese, Jovan Jose
Construction of high-dimensional neural network potentials based on atomic pairs
- PII-099. Fontineles, Tancredo
Can cryptolepine intercalation mode into DNA be predicted by a simple model and density functional theory?
- PII-100. Wojtulewski, Sławomir
Intramolecular double proton transfer reactions in sulphur analogues of the oxalic ACID-DFT, ab initio calculations and aim analyses
- PII-101. Csontos, Jozsef
On the convergence of factors contributing to the dissociation energy of chlorine
- PII-102. Joubert Doriol, Loic
An investigation of the photochemical ring-opening of benzopyran
- PII-103. Peng, Qian
Vibration correlation function formalism of phosphorescence spectrum and intersystem crossing transition rate for complex molecules--- Duschinsky rotation effect
- PII-104. Baeck, Kyoung Koo
Ultrafast non-adiabatic photo-dynamics of small molecules: effects of initial vibration level and isotope substitution
- PII-105. (Previous PI-187) Kobayashi, Masato
Linear-scaling divide-and-conquer method for non-linear optical property calculations
- PII-106. Kovács, Gábor
Hydroamination of alkynes with ammonia catalyzed by gold-carbene complexes
- PII-107. Eriksson, Emma
Sarco(endo)plasmic reticulum Ca²⁺ ATPase (SERCA) is a possible target for hypericin
- PII-108. Bochenkova, Anastasia
Dichotomic branching in two-excited-state dynamics in the meta-chromophores of the green fluorescent protein
- PII-109. Ferro, David
Atoms in molecules interpretation of the Z effect at sp² centers
- PII-110. Urieta, José S.
Computational electrochemistry: oxidation potential for tert-butyl diethylcarbamate
- PII-111. Sánchez-Lozano, Marta
Computational study of progressive hydration of amines in gas phase
- PII-112. Díaz-Tendero, Sergio
Density functional theory study of organocatalytic additions of β-ketosulfoxides to conjugated aldehydes
- PII-113. Haya, Luisa
Quantum-chemical predictions of the reactivity of 1-tert-butyl 2-methyl pyrrolidine-1,2-dicarboxylate
- PII-114. Fjermestad, Torstein
Unprecedented observation of AuCl₃ as a source of chloronium ions
- PII-115. Silva Jr, Humberto
Charge transfer and fragmentation in C₆₀+C⁶⁺ collisions
- PII-116. Cortona, Pietro
New hybrid functionals for density-functional electronic-structure calculations
- PII-117. Bochenkov, Vladimir
Modeling the optical properties of nanoholes in thin platinum films

- P11-118. Heverly-Coulson, Gavin
Regeneration of oxidised glutathione peroxidase mimics using thiols
- P11-119. Ramanantoanina, Harry
Density functional study of the Jahn-Teller distortion in C_{60}^-
- P11-120. Mayeux, Charly
Alkali metal ion affinities in the gas phase: complete basis set extrapolation methodology
- P11-121. Faginas Lago, Noelia
Molecular dynamics of NMA–NMA and NMA– H_2O aggregates using a portable intermolecular potential
- P11-122. Papadopoulos, Anastasios
Molecular orbital contributions to the induced magnetic field of benzene, cyclobutadiene, borazine, 1,2-, 1,3- and 1,4-azaborines
- P11-123. Temprado, Manuel
Computational study of the reaction mechanism of the oxidation of phosphines by nitrile oxides
- P11-124. Hénon, Eric
Study of PDE4 inhibitors: quantum mechanical molecular docking deployed in a grid using CONFIT
- P11-125. García-Meseguer, Rafael
Application of collective coordinates for the study of the haloalkane dehalogenase reaction
- P11-126. Falklöf, Olle
Determination of excited-state pK_a values from quantum chemical calculations
- P11-127. Belanzoni, Paola
Similarity and dissimilarity of hydroxylation by dinuclear methane monooxygenase and the ubiquitous mononuclear $Fe(IV)O^{2+}$ group
- P11-128. Sablon, Nick
Quantifying electron delocalisation
- P11-129. Siebert, Matthew
Elucidating enzyme influence in abietic acid biosynthesis through direct dynamics on a bifurcating potential energy surface
- P11-130. Sánchez-de-Armas, Rocío
Molecular modification of coumarin dyes for more efficient dye sensitized solar cells
- P11-131. Durbeej, Bo
Computational prediction of molecular rotor function in a protein
- P11-132. Espinal, Juan F.
DFT investigation of Li, Na, and K interactions with graphene layers
- P11-133. Mintz, Benjamin
Utilization of the MADNESS parallel runtime within the PSI4 computational chemistry software package
- P11-134. Carvalho, Silvia
Molecular recognition studies of the inhibition of a phospholipase A2 by NSAIDs
- P11-135. Zapata-Rivera, Jhon
Dioxygen activation by LM ($M = Cu, Ni$) complexes. Charge transfer and electronic structure
- P11-136. Aranda, Juan
Theoretical study of the reaction mechanism of adenine N5-methyltransferase M.TaqI
- P11-137. Cybulski, Hubert
Theoretical study of the pyridine–(helium) $_n$, $n = 1, 2$, van der Waals complexes
- P11-138. Daza, Martha Cecilia
Computational study of the electronic structure of thionine
- P11-139. Zimmermann, Tomas
Evaluation of the non(adi)abaticity of the quantum molecular dynamics using the dephasing representation of quantum fidelity
- P11-140. Salter-Duke, Brian J.
Valence bond theory – what insights does approaching the complete basis limit give us?
- P11-141. Yildirim, Asli
Modelling Ring-chain-ring Tautomerization of N-(o-aryl)-4-Hydroxy-2-oxazolidinone Derivatives

- PII-142. Nilsson Lill, Sten O.
DFT studies of the heck reaction
- PII-143. Agopcan, Sesil
Regioselectivity and stereoselectivity in intramolecular nitrene 1,3-dipolar cycloadditions to form a key intermediate in a histrionicotoxin synthesis
- PII-144. Flores-Morales, Patricio
Theoretical Studies of the Enhanced Reactivity of Lys182 in Glucose 6-Phosphate Dehydrogenase from Leuconostoc mesenteroides
- PII-145. Riley, Kevin
Energetics of Protein-Ligand Interactions Involving Halogen Bonds
- PII-146. Closser, Kristina
Local configuration interaction singles and applications to the excited states of helium clusters
- PII-147. Coiffier, Claire
Analysis of preferred conformations of c-furanosides by means of quantum mechanics approaches
- PII-148. Srinivasadesikan, Venkatesan
Computational investigations for the misincorporation of N^{2,3}-ethenoguanine adduct with DNA bases
- PII-149. Zinovjev, Kirill
QM/MM study of adenosine deaminase reaction mechanism
- PII-150. Esseffar, M'hamed
A DFT study of the role of the Lewis acid catalyst in the mechanism of the 1,3-dipolar cycloadditions of nitrile imines towards electron-deficient acryloyl derivatives
- PII-151. Kiewisch, Karin
Quantum-mechanical protein densities from subsystem-density functional theory
- PII-152. Roldán, Alberto
CO₂ activation catalyzed by inverse spinel iron sulfide
- PII-153. Dzade, Nelson
A DFT study of CO₂ adsorption on tetragonal iron sulfide (mackinawite)
- PII-154. Hedegård, Erik Donovan
Modified aug-cc-pVTZ basis sets for EPR Hyperfine Coupling Constants: First Transition Row Metals
- PII-155. Navarro, Armando
DFT benchmark for computation of long-range carbon-proton scalar coupling constants
- PII-156. Van Hemert, Marc
Stability of small aluminum clusters supported on graphene
- PII-157. Maréchal, Jean-Didier
Computational approaches for the prediction of the interactions of metallic species with protein: applications to artificial enzymes
- PII-158. Ruiz-Barragán, Sergi
Conical Intersection Optimization algorithms based on the Intersection Space Hessian
- PII-159. Teixeira, Osvaldo
Ab initio study of ClO₂ ground state. Towards a DMBE potential energy surface
- PII-160. Tamm, Toomas
Equilibria in conformationally flexible molecules
- PII-161. Mulet-Gas, Marc
Stability of Endohedral Metallofullerenes: Maximum Pentagon Separation Rule
- PII-162. Osadchuk, Irina
Computational modelling of Ti cyclopentanedione complexes
- PII-163. Roca-Sanjuán, Daniel
Are chemiluminescence and fluorescence related to the same emissive state? A CASPT2 study on a coelenteramide model
- PII-164. Fernandes, Kyle
Free energy hypersurfaces for the enzymatically catalysed isomerisation of chorismate to prephenate
- PII-165. Coe, Jeremy Patrick
Monte Carlo configuration interaction applied to excited states for photochemistry and spectroscopy

- PII-166. Chen, Jianming
Theoretical evaluation of thermoelectric figure of merit of phthalocyanine compounds
- PII-167. Vilella, Laia
Balancing Lewis Acidity and Brønsted Basicity for Optimal Catalytic Water Oxidation. A DFT Study
- PII-168. Alemany, Pere
Continuous Symmetry Measures: the Behaviour of Wavefunctions with Respect to the Irreducible Representations of a Symmetry Group
- PII-169. Barnett, Christopher
Ring pucker is central to transition state stabilisation in the glycosylation mechanism of cellobiohydrolase I
- PII-170. Addicoat, Matthew
Efficiency of an optimized Evolutionary Algorithm for locating Minimum Energy Conformers
- PII-171. Becker, Johannes
New program package for conformational search based on Tabu search: the CAST program
- PII-172. Gromov, Evgeniy
Ab initio study of photoinduced isomerization in the photoactive yellow protein (PYP) chromophore
- PII-173. Ortuño, Manuel Angel
Hydration pattern of trans-[PtCl₂(NH₃)(N-glycine)] provided by ab initio molecular dynamics simulations
- PII-174. Vysotskiy, Victor P.
The parallel electron propagator method and its application to anions
- PII-175. Frau, Juan
Avoiding gas phase calculations in theoretical pK_a predictions
- PII-176. Gamielien, Riedaa
Distance and orientational potential of mean force elucidates aromatic amino acid association – with implications to coarse-grained molecular dynamics
- PII-177. Bergès, Jacqueline
« Inverse hydration » of platinum complexes: theoretically predicted H-bond between H₂O and Pt(II) identified by neutron diffraction
- PII-178. Ortiz, Daniel
A combined experimental and DFT investigation of isomeric heparin disaccharides metal complexes
- PII-179. Garcia-Melchor, Max
A QM study on the origin of the enantioselectivity: the asymmetric Suzuki-Miyaura cross-coupling reaction
- PII-180. Balbuena, Perla
Confinement effects on reactivity
- PII-181. Le, Tu
Robust and predictive modelling of phase behaviour of nanostructured lipid-based self-assembled materials
- PII-182. Borschevsky, Anastasia
Benchmark Calculations of Atomic Properties of the 7p Elements
- PII-183. Francisco, Evelio
Interacting quantum atoms delocalization indexes evaluated with approximated second order reduced density matrices
- PII-184. Eskandari, Kiamars
The QTAIM properties of halogen atoms in halogen bonding
- PII-185. Castet, Frédéric
Supramolecular organization and charge transport properties of self-assembled pi–pi stacks of perylene diimide dyes
- PII-186. Lombardi, Andrea
Carbon dioxide collision dynamics: vibrational energy transfer
- PII-187. Roca, Maite
In search of dynamical recrossings to study the reversibility of a decarboxylation reaction
- PII-188. Ouk, Chanda-Malis
Ab initio Molecular Orbital calculations of the electronic structure for the CH₄ + N(²D) reaction and their implications for atmospheric models of Titan
- PII-189. Andrikopoulos, Prokopis C.
Examining the role of zeolitic oxygens during the N₂O decomposition

- PII-190. Domracheva, Tatiana
Photoinduced electron transfer in DNA repair enzymes photolyases: A computational study
- PII-191. Graña, Ana M.
Electron density analysis of methane...benzene complex by means of QTAIM. Comparing CCSD, M05-2X and MPW1B95 approaches
- PII-192. Melichercik, Miroslav
Effects of solvation on electron affinities of uracil
- PII-193 (previous PI-088) Tachikawa, Masanori
Path integral simulation for hydrogen bonded systems: protonic quantum nature and H/D isotope effect
- PII-194. Hernández-Laguna, Alfonso
DFT elastic properties of muscovite-paragonite series
- PII-195. Hargis, Jacqueline
What makes the "perfect penicillin" perfect?: identifying the nature of substrate specificity using hybrid QM/MM methodology
- PII-196. Formoso, Elena
Thio-effects on the solvation and enzyme-ligand interactions of RNase A – CPA complex
- PII-197. Carrazana-García, Jorge A.
Energetic analysis of the guanidinium–benzene interaction modulated by anions
- PII-198. Rodríguez-Sanz, Ana A.
Effect of stepwise microhydration on the methylammonium...phenol interaction
- PII-199. Campo-Cacharrón, Alba
Study of cation... π interactions modulated by the environment
- PII-200. Cabaleiro-Lago, Enrique M.
Study of the interaction of phenylalanine and guanidinium cation
- PII-201. Mironov, Vladimir
Photophysical properties of the kindling fluorescent protein
- PII-202. Ottonelli, Massimo
Density Functional Study of Electronic and Optical Properties of Large Silver Nanocage Clusters
- PII-203. Butchosa, Cristina
MS-CASPT2 study of hole transfer in guanine-tryptophan systems
- PII-204. Wilkinson, Karl
From games to GAMESS (-UK): GPU Acceleration of Integral evaluation
- PII-205. Gracia, Lourdes
The role of excited states in photoluminescence of CaWO₄ and SrTiO₃: An experimental and theoretical investigation
- PII-206. Fábri, Csaba
Toward the line list of methane
- PII-207. Szidarovszky, Tamás
Rovibrational spectra near dissociation
- PII-208. Grabowski, Sławomir
Ab Initio Calculations on NH₄⁺...(C₂H₂)_n Ammonium - Acetylene Clusters
- PII-209. Lorenzo, Isidro
Factors of stabilization of dimers of gallic acid with thymine and adenine
- PII-210. Zurek, Justyna
Ultrafast photoinduced stereochemistry and spectroscopy of closed and open shell transition metal complexes
- PII-211. Castillo, Raquel
Theoretical view of formate dehydrogenase mutations
- PII-212. Bordes, Isabel
Theoretical study of molecular mechanism of α , β - epoxyesters
- PII-213. García-Revilla, Marco
Chemical interactions from the profiles of the delocalization indexes
- PII-214. Coto, Pedro B.
Dynamical simulation of photoinduced electron transfer in self assembled monolayers at metal surfaces

- P11-215. Bokareva, Olga
Theoretical study of charge-transfer processes in [Ir(PPY)₂(BPY)]⁺ based system for photocatalytic water splitting
- P11-216. Valero, Rosendo
Density functional plane-wave study of raman and inelastic neutron scattering vibrational spectra of cis- and trans-diamminedichloroplatinum(II) and diamminedichloropalladium(II)
- P11-217. Settels, Volker
Ab initio study on excited states of aggregates of perylene based dyes
- P11-218. Gutiérrez-Oliva, Soledad
The Reaction Force Perspective: Theoretical Study of the Mechanism of Formation of Amino Acetonitrile in the Interstellar Medium.
- P11-219. Arcisauskaitė, Vaida
NMR shielding constants and chemical shifts in linear ¹⁹⁹Hg compounds: a comparison of three relativistic computational methods
- P11-220. Domingo, Luis Ramón
Theoretical study of the 1,3-dipolar cycloaddition reaction of carbonyl ylides with 1,2-diones
- P11-221. Chekirou, Nawel Leila
Theoretical study of the inclusion process between Tetracaine-β cyclodextrin and Procaine-β cyclodextrin type 1:1 and 1:2. A Comparative study
- P11-222. Ess, Daniel
Computational investigation of ligand lone-pair influence on alkane and arene metal-mediated C-H bond activation
- P11-223. Orozco, Yoelvis
Theoretical study of photophysical phenomena in 1-nitronaphthalene molecular system including methanol and ethanol solvent effects
- P11-224. Leverentz, Hannah
The multipole variational explicit polarization (X-Pol) potential
- P11-225. Iida, Kenji
Development of a 2D-RISM equation and its application to solid-liquid interface
- P11-226. Takano, Keiko
DFT study of Me/Cl exchange reaction on Pt complex with phosphine ligand
- P11-227. Höfener, Sebastian
Fluorescence behaviour of (selected) isoflavones
- P11-228. (Previous PI-222) Kus, Tomasz
An application of the charge stabilization technique in the double ionization potential Equation-of-Motion calculations
- P11-229. Mendes, Paulo
DFT studies on the NLO properties of ruthenium (II) thienyl complexes
- P11-230. Ugur, Ilke
Elucidation of the deamidation in triosophosphate isomerase (TIM) with molecular dynamics (MD)
- P11-231. Madhav, Vijay
Compliance constants in redundant internal coordinates and theoretical interpretation of gauche and cis effects
- P11-232. Sabolovic, Jasmina
MD modeling and kinetic effects of self-assembly of trans and cis bis(L-alaninato)copper(II) complexes into a crystallization nucleus in aqueous solution
- P11-233. Steinmann, Casper
The effective fragment molecular orbital method for covalent systems
- P11-234. Buchowiecki, Marcin
Direct evaluation of the temperature dependence of the rate constant based on the quantum instanton approximation
- P11-235. Sheu, Sheh-Yi
Determination of protein surface hydration shell free energy of water motion: theoretical study and molecular dynamics simulation
- P11-236. Yang, Dah-Yen
Hydrogen bonds in membrane proteins
- P11-237. Esterhuysen, Catharine
Distinguishing divalent Carbon(0) compounds from allenes by complexation to AuCl

- P11-238. Palyulin, Vladimir
Strain and conformational energies in some oxa- and thia-analogs of bicyclo[3.3.1]nonane
- P11-239. Kikuchi, Hiroto
Structure-based inhibitor mechanism of febuxostat for xanthine oxidoreductase: molecular dynamics study
- P11-240. Mazack, Michael
ACG: Analytical Coarse-Graining for Proteins
- P11-241. Šulc, Miroslav
Semiclassical calculation of ultrafast time-resolved electronic spectra
- P11-242. Matamala, Adelio
HOMO/LUMO energy levels of normal and branched benzo-catafusenes: a case study of molecular property transferability
- P11-243. Hanada, Norika
Ab Initio Fragment Molecular Orbital Study of Peroxisome Proliferator-Activated Receptor (PPAR) Pan Agonist
- P11-244. Wu, Qunyan
Quantum mechanics/ molecular mechanics (QM/MM) calculation of solid effects on the excited-state process of the 2,3-dicyano-5,6-diphenylpyrazine molecule
- P11-245. Tsunekawa, Naoki
Effectiveness of some approaches for ab initio free energy calculations using the parameterized force fields for sampling
- P11-246. Schlangen, Maria
C–N coupling in the gas phase: Amination of ethene by “bare” Ni(NH₂)⁺
- P11-247. Park, Heesoo
Molecular adsorption on graphene nanoribbon
- P11-248. Thomsen, Ditte Linde
Hydrogen abstraction reactions how modification of the reactants affect the electronic interactions
- P11-249. Frigerio, Francesco
Molecular dynamics Simulation of the thermal behavior of PCBM crystal structures
- P11-250. Ansorg, Kay
Cation- π Interaction In Biological Systems
- P11-251. Casasnovas, Rodrigo
Theoretical Study on carbon acidities of PLP Schiff Bases.
- P11-252. Delcey, Mickael
Beyond DFT for theoretical bioinorganic chemistry
- P11-253. Tai, Truong
How far can the phenomenological shell model be applied to doped lithium clusters Li_nX, X = Al and Si?
- P11-254. Polo, Victor
Molecular simulations on the solvation process of terpenoids using supercritical carbon dioxide
- P11-255. Pomelli, Christian Silvio
The supermolecular approach to model the organic reactivity in room temperature ionic liquids
- P11-256. Mück-Lichtenfeld, Christian
Geometries and intramolecular strain in cyclophanes using dispersion corrected DFT
- P11-257. Estévez, Carlos M.
Intermolecular interactions of cations and anions with dibenzo-p-dioxins, thianthrenes and dibenzopyrazines. Implications in the design of neutral molecular receptors
- P11-258. Masgrau, Laura
Computational chemistry in structural biology: substrate binding in mammalian 15-lipoxygenases
- P11-259. Enciso, Marta
Modulation of the folding free energy landscape by circular permutation
- P11-260. Improta, Roberto
The excited state decay in DNA components: Insights from quantum dynamical approaches
- P11-261. Ramalho, João
Mono and binuclear complexes for nonlinear optical switching: A DFT study

- P11-262. Aguilar, Javier
Ab-initio and direct dynamics study of the $i\text{-C}_3\text{H}_7\text{Cl} + \text{Na}^+$ reaction
- P11-263. Takayanagi, Masayoshi
Incipient structural relaxation process of photolyzed carbonmonoxy myoglobin: statistical analysis by perturbation ensemble method
- P11-264. Vanicek, Jiri
Efficient evaluation of accuracy of molecular quantum dynamics using dephasing representation
- P11-265. Yamazaki, Shohei
Multi-state CASPT2 study of the nonradiative decay mechanisms of uracil and its derivatives
- P11-266. Domínguez, José Luis
The effect of active site protonation state and solvent exposure on in silico ligand fragment search for BACE-1
- P11-267. Rodríguez-Otero, Jesús
Ab initio and DFT study of sumanene
- P11-268. Moughal Shahi, Abdul Rehaman
DNA photorepair mechanism by (6-4) photolyase: a QM/MM study
- P11-269. Pérez, Patricia
Theoretical analysis of substituted Diels-Alder reagents to determine the polar or non polar character of the reaction
- P11-270. Méreau, Raphaël
Modeling of electronic processes at TiO_2/TCNQ interface based electronic devices
- P11-271. Fong-Padrón, Ceila
Intermolecular forces and structures of ionic liquids in ion pairs and small clusters
- P11-272. Zalesny, Robert
On the role of anharmonicity in vibrational nonlinear optical response of π -conjugated donor-acceptor molecules
- P11-273. Karasulu, Bora
Photochemistry of thio-substituted flavin derivatives
- P11-274. Demel, Ondrej
Explicitly correlated Mukherjee's state-specific multireference coupled cluster method
- P11-275. Costa, Dominique
Biocompatibility at the Atomic Scale: Adsorption of Peptides on Stainless Steel Modeled by a Combined DFT and Classical Approach
- P11-276. Jerabek, Paul
Structure and Bonding Analysis of the Compounds YX-E-XY ($\text{E} = \text{C-Pb}$, $\text{X} = \text{B-Tl}$; $\text{Y} = \text{H, F, Cl}$) - new divalent Element(0) varieties
- P11-277. Lu, You
Excited-State Dynamics of Adenine in Water and in DNA
- P11-278. Chamorro, Eduardo
Chemical reactivity within the $[\text{N},\text{N}]$ representation of the spin-polarized density functional theory framework
- P11-279. Otyepka, Michal
Atomistic model of membrane anchored cytochrome P450 2C9 (CYP2C9) and membrane positions of CYP2C9 substrate/product establish possible access and egress pathways to/from CYP2C9 active site
- P11-280. Nénon, Sébastien
Theoretical study of electronic process at the ZnO/TTF interface
- P11-281. (Previous P11-161) Sändig, Nadja
An azobenzene derivative on the gold surface; polymorphism and isomerization
- P11-282. Lundberg, Marcus
Theoretical approaches to core-hole spectroscopy of transition metals
- P11-283. Dognon, Jean-Pierre
Theoretical chemistry study of encapsulated Xenon as an NMR Sensor for magnetic resonance imaging
- P11-284. Loerbroks, Claudia
A model for depolymerisation of cellulose
- P11-285. Schoenebeck, Franziska
Mechanistic studies in palladium-catalysis: solvent and additive effects on selectivity

- PII-286. Boulanger, Eliot
A general boundary potential for hybrid QM/MM simulations using Drude oscillator polarizable model
- PII-287. Morell, Christophe
Application of the electron density force to chemical reactivity
- PII-288. Oliveira, João
Conformational studies of β -oligomers through the use of local correlation methods and a continuum solvation model
- PII-289. Pruitt, Spencer
Computational studies of the 1,2,4-triazolium dinitramide class of ionic liquids
- PII-290. Fanourgakis, Georgios
Calculations of the viscosities of liquid water by molecular simulations with polarizable interaction potentials
- PII-291. Meghezzi, Hacene
Modeling of the synthesis reaction of substituted diazepines with the methods PM3 and DFT
- PII-292. Federic, Jozef
Molecular modelling of microsolvated ion pairs
- PII-293. Katouda, Michio
Linear scaling RI-MP2 calculations of large molecules: FMO, DC, AND MT based approaches
- PII-294. Nadler, Roger
CdSe quantum dots exposed to a time-dependent electric field: effect of basis set and functional on the absorption spectrum
- PII-295. Guillaumes, Laia
The formation of a new cycle due to two hydrogen bonds: RAHB by means of delocalization indexes
- PII-296. Furuncuoglu Özaltın, Tugba
Investigation of the topoisomerase-targeted anti-cancer drug molecules: ab-initio and molecular dynamics study
- PII-297. Ince, Hasan Huseyin
QM/MM study on the GTP hydrolysis in the elongation factor-Tu (EF-Tu)
- PII-298. Kampa, Mario
The Reaction Mechanism of [NiFe] Hydrogenases
- PII-299. Srivastava, Hemant Kumar
Modelling DNA minor groove binders: a benchmark study

POSTER SESSION III (PIII-1 to PIII-267)
Friday, July 22 - 11.30-13.30h (Faculty of Economy)

PIII-001. Andrada, Diego
DFT study of thermal 1,3-dipolar cycloaddition reactions between alkynyl metal(0) Fischer carbene complexes and 3h-1,2-dithiole-3-thione derivatives

PIII-002. Josa, Daniela
Analysis of the performance of DFT-D, M05-2X and M06-2X for studying $\pi \cdots \pi$ interactions

PIII-003. Bartkowiak, Wojciech
Electric dipole (hyper)polarizabilities of spatially confined diatomic molecules

PIII-004. Atars, Gleisy
Relationship between anti-wear performance and molecular properties of some transition metal complexes as lubricant additives

PIII-005. Ding, Yun
Investigation of h-BN/Rh(111) nanomesh interacting with water

PIII-006. Jurecka, Petr
Deriving force field dihedral angle parameters for simulations in aqueous environment

PIII-007. Viciano, Ignacio
DFT/MM studies about the first hydroxylation step of Cytochrome P450 aromatase

PIII-008. Kocman, Mikulas
What is the role of graphene quadrupole moment in its intermolecular interactions?

PIII-009. Taylor, Daniel
Correlated calculations of the excited states of small molecules.

PIII-010. Vladimirova, Ksenia
Systematic analysis of coulomb-attenuated exchange- functional performance on excitation energies

PIII-011. Talman, James
Numerical methods for molecular orbitals

PIII-012. Zgarbova, Marie
Refinement of the glycosidic torsion profile based on high quality quantum chemical calculations

PIII-013. Schwarzer, Martin Christoph
Chemical Bonding in Pincer-Complexes of Group 2 and 4 Elements

PIII-014. Meana-Pañeda, Rubén
Accurate evaluation of partition functions for nonseparable two-dimensional hindered internal rotors

PIII-015. Meliá, Concepción.
Metallo- β -lactamases. a theoretical study of hydrolysis of β -lactam antibiotics

PIII-016. Barberot, Chantal
Primary amine addition to an unsaturated bromoderivative of levulinic acid: a computational study

PIII-017. Iron, Mark
Towards high accuracy calculation of pKa values

PIII-018. Bergendahl, Lisa Therese
Two-photon absorption in porphycenic macrocycles

PIII-019. Eliav, Ephraim
Electronic structure of relativistic quantum dots

PIII-020. Herrera, Barbara
On the description of the reactivity of azo compounds: electrostatic potential, average ionization energy and dual index

PIII-021. Bredtmann, Timm
Analysis of coupled electronic and nuclear dynamics induced by ultrashort laser pulses: Quantum simulations for the Cope rearrangement of semibullvalene

PIII-022. Martín, María Elena
Solvent effects in the absorption spectrum of a model of the rhodopsin chromophore

PIII-023. Sánchez Mendoza, María Luz
An ASEP/MD study of the structure and properties of ionic liquids

- P111-024. Savoyant, Adrien
Geminate hole-electron pair dissociation at Pentacene/C₆₀ interface
- P111-025. Groenewald, Wilma
Assessment of the factors that determine conformational preferences in mycolic acids from mycobacterium tuberculosis
- P111-026. Whittleton, Sarah
The effects of Ge and Al substitutions on the local geometries and NMR parameters of zeolite beta polymorph C
- P111-027. Swang, Ole
Rock'n'roll at gold: dynamics of a BPY-AuCl₃ complex
- P111-028. Salvador, Pedro
Calculation of Local Spins from Physical Space Analysis
- P111-029. Condic-Jurkic, Karmen
The protonation states of histidines in the active site of (6-4) photolyase
- P111-030. Homem-de-Mello, Paula
A Density Functional Study on Pb(II)-DPKSH complexes
- P111-031. Groves, Michael
Examining in situ the oxygen reduction reaction using density functional theory as a function of catalyst support
- P111-032. Naderi, Fereshteh
Complexes of a bio-molecule and a C₃₆ cage
- P111-033. Pittner, Jiri
A TDDFT study of absorption and fluorescence spectra of PRODAN in phospholipid membranes
- P111-034. Habershon, Scott
Classical and quantum free energy calculations for flexible water models
- P111-035. Saurí, Vicenta
Excited-state hydrogen/proton transfer processes in the guanine-cytosine base pair
- P111-036. Goto, Hitoshi
Improvement of four-body statistical pseudo-potential for native and mutated protein conformations
- P111-037. Havenith, Remco
The many-electron band structure approach: theory and application
- P111-038. Mosquera, Ricardo
Electronic interpretation of conformational preferences in benzyl derivatives
- P111-039. Anglada, Josep M.
Electronic and geometric features of the HO₂⁻ anion
- P111-040. Raynaud, Christophe
Unusual structures of tetracoordinated d⁴ ML₄ complexes: structural dependence on ligands and metal
- P111-041. Zalazar, María Fernanda
Nature of the adsorbate-catalyst interactions in the zeolite chemistry. A study based on the electron charge density
- P111-042. Azriel, Vladimir
Trajectory simulation of the dynamics of interaction in system KJ + Xe
- P111-043. Alzate-Morales, Jans H.
Exploring the use of QM/MM hybrid methods in the prediction of protein-ligand binding affinities
- P111-044. Rajchel, Lukasz
Separating intra- and intermonomer correlation in DFT-based description of intermolecular forces
- P111-045. Patchkovskii, Serguei
Electron currents from Born-Oppenheimer wavefunctions
- P111-046. Silva López, Carlos
Computational exploration of the five-bond-breaking catalytic mechanism
- P111-047. Rönnholm, Petra
Computational studies of chiral lithium N,P-amide complexes.
- P111-048. (Previous PI-046) Mammìno, Liliana
Acyphloroglucinols: overview of the results of a systematic computational study

- PIII-049. Johnson, Erin
Effects of Atomic Environment on Dispersion Coefficients
- PIII-050. Lucas, Maria De Fátima
Electron Transfer Pathways in Cytochrome c Oxidase
- PIII-051. Aquilante, Francesco
A mean-field approach to nonbonded interactions, away from empiricism and scaling walls
- PIII-052. Alves, Tiago Vinicius
Isomers on the $^1[H_4, C, S]$ potential energy surface: A CCSD(T) investigation
- PIII-053. Isborn, Christine
QM, MM, and QM/MM hydration free energies and solvatochromism with accelerated calculation of ground and CIS/TDDFT excited states using GPUs
- PIII-054. Shao, Yihan
Q-Chem 4.0
- PIII-055. Melaccio, Federico
QM/MM study of the initial photochemical events in Anabaena sensory rhodopsin
- PIII-056. Laurent, Adele
Characterization of coupled cis-trans isomerization and proton transfer in the photoactive yellow protein chromophore
- PIII-057. Ichikawa, Kazuhide
Atomic shell structure study by kinetic energy density and stress tensor density
- PIII-058. Fontineles, Tancredo Augusto
Can cryptolepine intercalation mode into DNA be predicted by a simple model and density functional theory?
- PIII-059. Ruedenberg, Klaus
A priori identification of configurational deadwood
- PIII-060. Shi, Qiang
Simulation of Quantum Dynamics in Condensed Phase Using the Hierarchical Equations of Motion Method
- PIII-061. Silva, Daniel
The effect of the aqueous environment on the one- and two-photon absorption of coumarin 120: A study using the S-QM/MM methodology and the ZINDO method
- PIII-062. Klobukowski, Mariusz
Model Core Potential Studies of Radon Chemistry
- PIII-063 (Previous PI-134) Simon, Aude
Atoms (Fe, Si) molecules (H₂O) and clusters on the surface of PAHs: molecular dynamics simulations
- PIII-064. Schapiro, Igor
Studying the photoisomerization mechanism in complex environments using QM/MM dynamics
- PIII-065. Tokoyama, Hiroaki
Finding crystal structures by the scaled hypersphere search method: acceleration of the automated search using DFTB+
- PIII-066. Mori, Hiroto
Ab initio fragment molecular orbital-molecular dynamics (FMO-MD) simulation on hydrolysis of anticancer platinum complexes
- PIII-067. Yamakado, Hideo
A method of automated search for crystal structures - New structures of carbon crystal
- PIII-068. Deshmukh, Milind
Highly accurate approximate method for binding energy of van der Waals complexes
- PIII-069. Murakami, Tatsuhiro
Theoretical study of photo-physical properties of indolylmaleimides
- PIII-070. Wang, Dong
Molecular dynamics simulations of host-guest interactions of α -cyclodextrin with an azobenzene-containing surfactant
- PIII-071. Baric, Danijela
Glycerol as a substrate and inactivator of B₁₂-dehydratases – a QM/MM study
- PIII-072. (Previous PI-154) Peran, Nena
Polycyano derivatives of some cyclic and polycyclic hydrocarbons provide stable anions and dianions – a density functional study

- PIII-073. Gierschner, Johannes
Exciton transport and injection in supramolecular nanostructured assemblies
- PIII-074. Cho, Yeonchoo
Fano resonance-based DNA sequencing
- PIII-075. Caballero, Marc
Thermal reactions induced by terahertz radiation
- PIII-076. Marsden, Colin
US₂²⁺ is not "thio-uranyl"!
- PIII-077. Zhao, Hailiang
DFT and ab initio study of metal corroles (Metal = Co, Fe, Mn)
- PIII-078. Preto, Marco
Machine learning techniques as a tool to correlate antioxidant activity with phenolic composition of natural extracts
- PIII-079. Diefenbach, Martin
Quantum chemical assessment of the bond energy of CuO⁺
- PIII-080. Radchenko, Eugene
Design of selective and safe organophosphorus inhibitors of serine esterases
- PIII-081. Khartabil, Hassan
New isothiazolone derivatives obtained by a Diels-Alder cycloaddition: a theoretical study
- PIII-082. Kayik, Gülru
A DFT study of stereospecific free radical polymerization of acrylamide derivatives
- PIII-083. Pasha, Farhan
DFT analysis for the impact of co-catalyst (MAO) over reaction profile of alkene oligomerization
- PIII-084. Nakayama, Akira
Ultrafast deactivation channel of electronically excited states of diphenyl and triphenyl methane dyes
- PIII-085. Muya, Tshishimbi
Boron fullerenes: stability, bonding analysis and chemical reactivity
- PIII-086. Makshakova, Olga
Study of geometry and vibrational spectra of helical polypeptides and their complexes with water and organic molecules
- PIII-087. Valdés, Álvaro
Translation-rotation energy levels of one H₂ molecule inside the three cages of the structure H clathrate hydrate
- PIII-088. (Previous PI-173) Antol, Ivana
The influence of multiple fluorination on alleged valence isomerisation of [2.2.2]propellanes
- PIII-089. Kazemi Babaheydari, Ali
Adsorption properties of NO on (6,0) and Al-doped (6,0) zigzag single-walled carbon nanotubes (CNTs) A density functional study
- PIII-090. Šebera, Jakub
DFT study of glycosidic bond cleavage of 8-oxoguanosine catalyzed by the human DNA repair protein hOGG1
- PIII-091. Feria, Leticia
CO Oxidation and WGS Reactions on Inverse CeO_x/Cu(111) Catalysts: A Density Functional Theory Study
- PIII-092. Safont, Vicent Sixte
Modeling the O1 radical route of the artemisinin decomposition process: a topological study
- PIII-093. Viegas, Luis Pedro
Catalytic role of water on the HO₂+nH₂O+O₃ reactive clusters
- PIII-094. Asensio, Amparo
Theoretical Study on the Reactivity of Sulfinil Imines with CF₃TMS/TBAT
- PIII-095. Pérez-Mondéjar, Vicente
On the role of the triplet state in the cis/trans isomerization of rhodopsin
- PIII-096. Coulaud, Esther
Theoretical study of magnetic exchange mechanisms: Application in bis-nitroxides
- PIII-097. Patel, Chandan
QM/MM-MD Investigations on Formation of Complex Oxidative DNA Defects

- PIII-098. Krasinski, Grzegorz
Molecular docking and DFT studies of the enzyme-catalyzed kinetic resolution
- PIII-099. Cypryk, Marek
Polymerization and copolymerization of L-lactide and ϵ -caprolactone
- PIII-100. Walker, Victoria
A Computational Investigation of Nitric Oxide Induced Oxidation of Oxyhemoglobin
- PIII-101. Bjoernsson, Ragnar
A QM/MM approach to Model Molecular Crystals: Local Geometry Optimization and NMR Properties
- PIII-102. (Previous PI-177) Martín-Martínez, Francisco J.
Aromaticity patterns on finite-length carbon nanotubes
- PIII-103. Rokob, Tibor András
Second order correction scheme for microiterative QM/MM optimizations using electrostatic embedding
- PIII-104. Catak, Saron
Competitive pathways for peptide deamidation
- PIII-105. Reis, Renata A. G.
Influence of ionic strength on structural dynamics of protein calgranulin C (S100A12)
- PIII-106. Domin, Dominik
Assessing spin-component scaled MP2 theory using anharmonic frequencies
- PIII-107. Goetze, Jan Philipp
Modelling the Photophysics of 1-deaza-flavin in Water: A Theoretical Study
- PIII-108. Zaleski-Ejgierd, Patryk
The very heavy and the very light: high pressure stabilization and emergent forms of PbH_4
- PIII-109. Brkljaca, Zlatko
Conformational study of small peptides and their circular dichroism spectra
- PIII-110. Milicevic, Zoran
The ordering of water around hydrophobic solutes in electric fields
- PIII-111. Geng, Caiyun
The C-H bond activation by diiron complexes with cyclic hydrogen bond
- PIII-112. Roos, Katarina
Theoretical modeling of ribonucleotide reductase - diiron, dimanganese or mixed
- PIII-113. Wang, Bo-Cheng
The Geometry Effects of Boron-Nitride Nanoribbons
- PIII-114. Schmidt, Thomas
Beyond the Lock and Key Principle
- PIII-115. Milián Medina, Begoña
Backbone flexibility in substituted polythiophenes
- PIII-117. Labet, Vanessa
A fresh look at dense hydrogen under pressure – evolution of the H--H distances
- PIII-118. Ramírez, Beatriz
DFT study of the unimolecular dehydrogenation kinetics of cyclohexadienes in gas phase
- PIII-119. Banas, Pavel
Performance of the molecular mechanics force fields for simulations of RNA hairpin loops
- PIII-120. Valdés, Haydee
Reductases of the truncated hemoglobin N (trHbN) from Mycobacterium tuberculosis
- PIII-121. El Khatib, Muammar
On the electronic structure of cyclic oligocenes
- PIII-122. Rudbeck, Maria
Driving through a phosphate cycle
- PIII-123. Minenkov, Yury
The initiation kinetics of Grubbs ruthenium-based olefin metathesis catalysts

- PIII-124. González-Lafont, Àngels
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- PIII-125. Lee, Shyi-Long
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