GUI, CRYSTAL, solid state

CRYSPLOT is a web-based graphical tool used to visualize physical and chemical properties of periodic systems. Through its web page, users can easily plot different properties as band structure, density of states, electron charge density maps, simulated IR/Raman spectra, and as computed with the CRYSTAL code. The article by G. Beata, G. Perego and B. Civalleri on page 2329 describes what it does and how it works, with selected applications taken from the study of metal-organic frameworks. DOI: 10.1002/jcc.25858

Coming Soon

Computational assessment of MLCT vs. MC stabilities in first-to-third row d^6 pseudo-octahedral transition metal complexes
Aymerick Batlogg and Maria Fumanal

Excited state analysis of a first (Mn-), second (Ru-) and third (Re-) row d^6 pseudo-octahedral transition metal complex, each displaying a different metal-to-ligand charge-transfer (MLCT) vs. metal-centered (MC) potential energy landscape. Time-dependent density functional theory (TDDFT) and wave function-based methods (MS-CASPT2) are evaluated with respect to the choice of the reference geometry. The results question the validity of assessing DFT/TDDFT performance via direct comparison with MS-CASPT2 at the same DFT reference geometry as a standard strategy. DOI: 10.1002/jcc.26014

Controlled-Advancement Rigid-Body Optimization of Nanosystems
Petr Popov, Sergei Grudinin, Andrey Kurdyuk, Pavel Buslaev, and Stephane Redon

Conformational space along with the energy function gives rise to the energy landscape, which typically has many local minima and maxima. Optimization over such a landscape is full of pitfalls and requires well-tuned parametrization of the optimization method. Controlled advancement optimization allows to avoid these pitfalls, by considering only relevant molecular displacements in the conformational space. In this study we propose novel optimization method that remains stable, regardless the complexity of the energy landscape. DOI: 10.1002/jcc.26016
Nine Questions on Energy Decomposition Analysis
Juan Andrés, Paul W. Ayers, Roberto A. Boto, Ramon Carbó-Dorca, Henry Chemet, Jerzy Cioslowski, Julia Contreras-García, David L. Cooper, Gernot Frenking, Carlo Gatti, Famaz Heidar-Zadeh, Laurent Joubert, Ángel Martín Pendás, Eduard Matito, István Mayer, Alston J. Misquitta, Yirong Mo, Julien Pilmé, Paul L. A. Popelier, Martin Rahm, Eloy Ramos-Cordoba, Pedro Salvador, W. H. Eugen Schwarz, Shant Shahbazian, Bernard Silvi, Miquel Solá, Krzysztof Szalewicz, Vincent Tognetti, Frank Weinhold, and Émilie-Laure Zins

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Rational Design of Electronically Labile Dinuclear Fe and Co complexes with 1,10-Phenanthroline-5,6-Diimine: A DFT study
Alyona A. Starikova, Maxim G. Chegerev, Andrey G. Starikov, and Vladimir I. Minkin

Published online 22 June 2019

Superhalogen and Superacid
Andrey V. Kulsha and Dmitry I. Sharapa

Published online 29 June 2019

Magnetic Signatures of Hydroxyl- and Water-Terminated Neutral and Tetra-Anionic Mn₁₂-Acetate
Javaria Batool, Torsten Hahn, and Mark R. Pederson

Published online 3 July 2019

Many methods enable the calculation of contributions to the interaction energy between two fragments of a molecular or complex system.

The performed DFT modeling of the isomeric forms of a series of homo- and heterometallic complexes of 1,10-phenanthroline-5,6-diamine with Co(II) bis-diketonates and Fe(II) dihydrobis (pyrazolyl)borates has provided insights into dependence of electronic states and magnetic properties of the systems under study on their structural peculiarities. The computational findings allowed to reveal magnetically-active compounds capable of undergoing thermally-initiated spin-state switching rearrangements.

A fluorine atom is encapsulated into a dodecahedrane cage decorated with 20 cyano groups. The resulting superhalogen has electron affinity of 10.8 eV, forming a very non-nucleophilic anion of $I_h$ symmetry with gas-phase basicity of just 208 kcal/mol.

The field strengths associated with resonant tunneling of magnetization in Mn-Acetate and other molecular magnets are extremely sensitive to changes in their charge state, chemical composition, or ligand substitution. Density-functional calculations, with self-interaction corrections, are used to show that this water-containing molecule behaves as an all-in-one nanoreactor and observatory, in waiting, and effectively allows for quantum sensing of water molecule decomposition under exposure to additional electrons.
The Polarizable Continuum Model helps in determining the experimental electric dipole moment of molecules in solution.

The bonding character of noncovalent noble-gas (Ng) complexes peculiarly emerges by analyzing the electron energy density $H(r)$. Particularly, informative is the dashed region signed by the arrow. In the presence of a ligand, its size and shape, truly spherical in any free Ng atom, undergoes changes that mirror the relative role of dispersion, induction, and charge transfer. The presently proposed degree of polarization measures these changes, and is, therefore, a quantitative index of bonding character.

Software News and Updates

CRYSPLOT is a publicly accessible web-based tool (http://crysplot.crystalsolutions.eu) to visualize physico-chemical properties of periodic systems (i.e., crystals, surfaces and polymers) as computed with the CRYSTAL code. It has been designed as a very intuitive graphical tool, a low entry-level interface, to all types of users, from beginners to experts, and purposes, from education to research, as shown with selected examples.

An out-of-the-box, stand-alone program package MLatom with a user-friendly online manual is presented for computationally efficient atomistic simulations with machine learning. MLatom supports kernel ridge regression, various sampling procedures including structure-based sampling, model selection and evaluation, and conversion of molecular coordinates to several built-in molecular descriptors. The program can be used for solving generic machine-learning tasks, constructing molecular potential energy surfaces and calculating energy gradients, and exploring chemical space.

Erratum

Exploring the Structure and Stability of Cholesterol Dimer Formation in Multicomponent Lipid Bilayers

Asanga Bandara, Afra Panahi, George A. Pantelopulos, and John E. Straub

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