Introduced by Xie and coworkers on page 541, SMPBS (smpbs.math.uwm.edu) is a web server for computing and visualizing biomolecular electrostatics using finite element solvers of the size modified Poisson-Boltzmann equation (SMPBE). SMPBS features an interactive, hardware-accelerated molecular visualization viewer, based on the 3Dmol.js library, that allows computed electrostatics to be directly mapped onto an irregular triangular mesh of a molecular surface. The interface also enables efficient calculation of electrostatic solvation and binding free energies. Furthermore, SMPBE efficiently allows minimizing a new objective electrostatic free energy subject to an ionic size constraint, and thus can be used as a more versatile substitute for classic PBE.

Automated First-Principles Mapping for Phase-Change Materials
Marc Esser, Stefan Maintz, and Richard Dranskowski
A first-principles “treasure map” is presented which predicts seven novel synthetic targets for phase-change materials as rewritable data-storage media. The map is constituted by heuristical descriptors that analyze the bonding situation within the solids in terms of ionicity and orbital mixing, and these descriptors also include crucial structural information. By doing so, the newly developed coordinates place materials with similar physical properties into similar map areas, thereby creating a “phase-change island”.

DOI: 10.1002/jcc.24724

ForConX - A Forcefield Conversion Tool Based on XML
Christian Schroeder et al.
A general tool for the force field conversion on the basis of an XML document is presented. The force field is converted to and from the XML structure facilitating the implementation of new Molecular Dynamics programs for the conversion. Furthermore, the XML structure is human readable and can be manipulated before continuing the conversion.

DOI: 10.1002/jcc.24708
The Orbital-weighted Fukui function ($\nu_w(r)$) and its topological analysis are proposed as a simple yet effective new local reactivity model. This model takes into account contributions from all orbitals, for which densities are weighed according to a Gaussian-function centered at the chemical potential value. This strategy proves to be a simple way to improve the Fukui function in cases where there is a degeneracy or quasi-degeneracy of frontier orbitals on the neutral, cation, or anion of the studied molecule. The model shows to be effective (assessed by a region selectivity analysis of a set of aromatic molecules) where other Frontier Molecular Orbital theory-based approximations have failed.

A massively parallel algorithm of the analytical energy gradient calculations based on the resolution of identity Møller–Plesset perturbation (RI-MP2) method from the restricted Hartree–Fock reference is developed for geometry optimization calculations of large molecules using supercomputers. The analytical energy gradient calculation of Trp-cage protein 1L2Y at the RI-MP2/def2-SVP level is speeded up considerably enough to perform the geometry optimization using the new algorithm and implementation on the K computer.

Force field parameterization is a highly dimensional optimization problem and an exhaustive search of parameter space is computationally too costly. This article shows that by a systematic evaluation of subsets of parameters, we can efficiently optimize transferable parameters based on relevant physico-chemical compound properties for the complete nearby parameter space.

Here, we assess the accuracy of various approaches implemented in Vienna \textit{ab initio} simulation package to estimate core-level binding-energy shifts ($\Delta$BEs) using projector-augmented-wave method to treat core electrons. Different exchange-correlation functionals within density functional theory are tested on a 68 molecules dataset accounting 185 different 1$s$ ($\Delta$BEs) for which experimental data is available. Janak–Slater transition state approach yields an accuracy similar to all electron \textit{D}SCF calculations, and close to X-ray photoemission accuracy of 0.1 eV.
**Full Papers**

Density Functional Theory calculations evidence the effect of relativistic effects on bandgap estimations of semiconductors, as evidenced on stoichiometric and reduced ZnO where bandgap is reduced by 0.25 eV, according to PBE0 results using a numerical atomic orbital basis set.

Electronic Structure of Stoichiometric and Reduced ZnO from Periodic Relativistic All Electron Hybrid Density Functional Calculations Using Numeric Atom-Centered Orbitals

Francesc Viñes and Francesc Illas

Published online 11 January 2017

A detailed density functional theory (DFT) study involving ionic liquids is presented, where it is shown that it is necessary to introduce dispersion correction to get significant improvements in geometries, accurate interaction energies, and self-interaction error correction is necessary for charges and dipole moments in the ionic pair. Geometries of ionic pairs obtained at DFT level are extensively used to predict properties through theoretical methods.

The Role of Errors Related to DFT Methods in Calculations Involving Ion Pairs of Ionic Liquids

Isabel Lage-Estebanez, Lourdes del Olmo, Rafael López, and José Manuel García de la Vega

Published online in Wiley Online Library

**Software News and Updates**

SMPBS (smpbs.math.uwm.edu) is a web server for computing and visualizing biomolecular electrostatics using finite element solvers of the size modified Poisson-Boltzmann equation (SMPBE). It features an interactive, hardware-accelerated molecular visualization viewer, based on the 3Dmol.js library, that allows computed electrostatics to be directly mapped onto an irregular triangular mesh of a molecular surface. It also enables efficient calculation of electrostatic solvation and binding free energies. Furthermore, SMPBE is shown to be optimal in the sense of minimizing a new objective electrostatic free energy subject to an ionic size constraint, and can be a more versatile substitute for classic PBE.

SMPBS: Web Server for Computing Biomolecular Electrostatics Using Finite Element Solvers of Size Modified Poisson-Boltzmann Equation

Yang Xie, Jinyong Ying, and Dexuan Xie

Published online 4 January 2017

In this article, implementation of steered molecular dynamics in coarse-grain UNited RESidue (UNRES) force field is presented. Two variants of steered molecular dynamics have been implemented: with a constant force and a constant velocity.

Introduction of Steered Molecular Dynamics into UNRES Coarse-Grained Simulations Package

Adam K. Sieradzan and Rafał Jakubowski

Published online 11 January 2017

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