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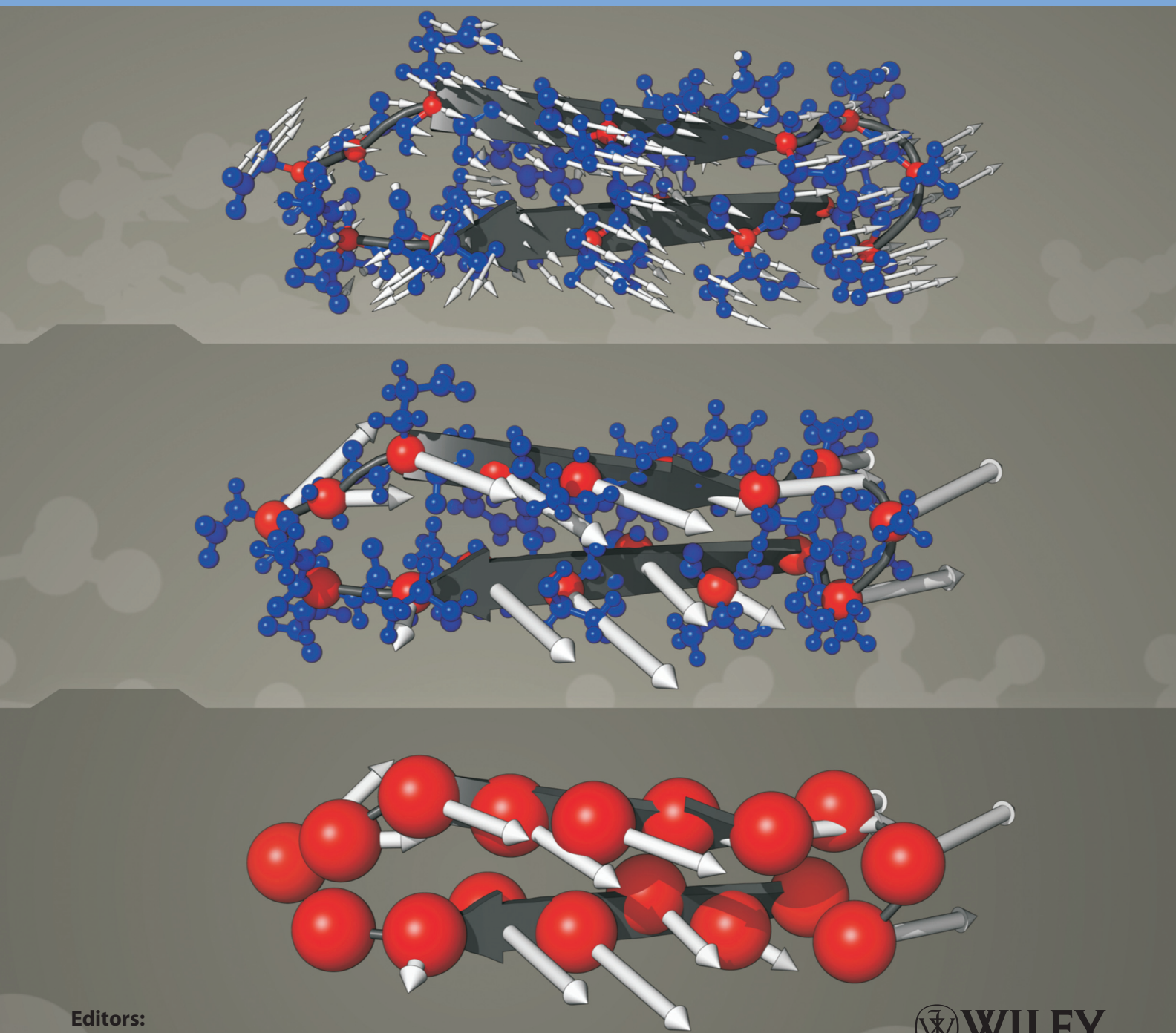

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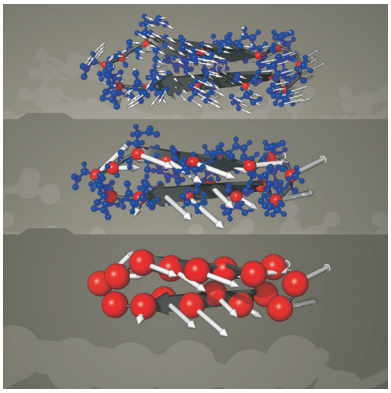
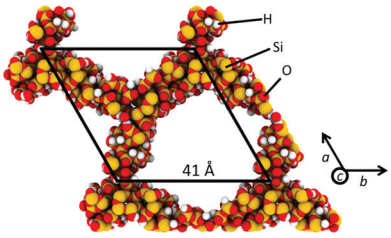


Hessian Reduction Versus Coarse-Graining

The cover shows the discrepancy in the number of displacements between all-atom models (top) and coarse-grained models (bottom). The work by An Ghysels, Benjamin T. Miller, Frank C. Pickard IV, and Bernard R. Brooks on page 2250 develops a methodology to derive "imploded" models from the all-atom representation, with the same amount of displacements as the coarse-grained model (middle figure).



Massive Parallel CRYSTAL

The performance of the massive parallel version of CRYSTAL09 has been studied on different HPC architectures for mesoporous silica MCM-41, a system consisting of a large primitive cell (41 × 41 × 12 Å) with 579 atoms ($H_{102}O_{335}Si_{142}$) and no point symmetry, as presented by Roberto Dovesi and colleagues on page 2276. MCM-41 is characterized by a long range ordered network of hexagonal pores and amorphous walls at short range. B3LYP/6-31G(d,p) full converged SCF plus gradient calculations on up to 1 × 1 × 10 MCM-41 supercells (5790 atoms) have been performed with up to 2048 cores on three different HPC architectures, showing that runs with up to 100000 AOs are now feasible.

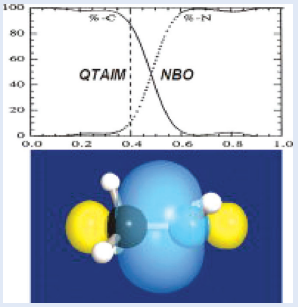
Coming Soon

Look for these important papers in upcoming issues

Natural Bond Critical Point Analysis: Quantitative Relationships Between Natural Bond Orbital-based and QTAIM-based Topological Descriptors of Chemical Bonding

F. Weinhold

A new NBO-based program displays the intimate connections between quantum theory of atoms in molecules (QTAIM) bond critical points and corresponding localized natural bond orbitals (NBOs), delocalized MOs, or other orbital-type contributions to total electron density.
DOI: 10.1002/jcc.23057



Natural Bond Orbital Analysis: A Critical Overview of Relationships to Alternative Bonding Perspectives

F. Weinhold

A conceptual overview of natural bond orbital theory is provided, including critical discussion of its many points of comparison and contrast with alternative valence bond, molecular orbital, and quantum theory of atoms in molecules conceptions of chemical bonding interactions.
DOI: 10.1002/jcc.23060