ADDENDUM: Fall, 2006 Newsletter of the Theoretical Chemistry Subdivision

Announcement concerning the Fall, 2006 San Francisco national meeting of the ACS: submitted by John McKelvey

> There will be a Symposium in COMP, and co-sponsored by the Physical Division, "DFTB: An Approximate Density Functional Method." DFTB can be thought of as an addition to the EHT method. where DFT coulombic and exchange functionals have been added, and the procedure then parameterized against the PBE functional. To name one major benefit, speed is comparable to MOPAC, and accuracy in geometries comparable to B3LYP, at least in my hands, in both ground state and excited state applications.
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> There are 38 talks over Mon-Wed AM and PM, and also 4 posters.
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> The other two Organizers are Thomas Frauenheim and Marcus Elstner, co-developers of the SCC-DFTB codes.