C3.13 (Ch. Jacob)

[C3.13:1] ‡ S. Fux, Ch.R. Jacob, J. Neugebauer, L. Visscher, and M. Reiher, *Accurate frozen-density embedding potentials as a first step towards a subsystem description of covalent bonds*, J. Chem. Phys. **132**, 164101 (2010)

[C3.13:2] ‡ V. Liégeois, Ch.R. Jacob, B. Champagne, and M. Reiher, *Analysis of vibrational Raman optical activity signatures of the $(TG)_N$ and $(GG)_N$ conformations of isotactic polypropylene chains in terms of localized modes*, J. Phys. Chem. A **114**, 7198 (2010)

[C3.13:3] ‡ T. Weymuth, Ch.R. Jacob, and M. Reiher, *A local mode model for understanding the dependence of the extended amide III vibrations on secondary structure*, J. Phys. Chem. B **114**, 10649 (2010)

[C3.13:4] ‡ T. Weymuth, Ch.R. Jacob, and M. Reiher, *Identifying protein β-turns with vibrational Raman optical activity*, ChemPhysChem **12**, 1165 (2011)

[C3.13:5] ‡ Ch.R. Jacob, S.M. Beyhan, R.E. Bulo, A.S.P. Gomes, A.W. Götz, K. Kiewisch, J. Sikkema, and L. Visscher, *PyADF – A scripting framework for multiscale quantum chemistry*, J. Comput. Chem. **32**, 2328 (2011)

[C3.13:6] ‡ N.S. Bieler, M.P. Haag, Ch.R. Jacob, and M. Reiher, *Analysis of the Cartesian Tensor Transfer Method for Calculating Vibrational Spectra of Polypeptides*, J. Chem. Theory Comput. **12**, 1867 (2011)

[C3.13:7] ‡ S. Fux, Ch.R. Jacob, J. Neugebauer, L. Visscher, and M. Reiher, *Response to Comment on 'Accurate frozen-density embedding potentials as a first step towards a subsystem description of covalent bonds'*, J. Chem. Phys. **135**, 027102 (2011)

[C3.13:8] ‡ K. Boguslawski, Ch.R. Jacob, and M. Reiher, *Can DFT accurately predict spin densities? Analysis of discrepancies in iron nitrosyl complexes*, J. Chem. Theory Comput. **7**, 2740 (2011)

[C3.13:9] Ch.R. Jacob, *Theoretical study of the Raman optical activity spectra of 310-helical polypeptides*, ChemPhysChem **12**, 3291 (2011)

[C3.13:10] Ch.R. Jacob, *Unambiguous optimization of effective potentials in finite basis sets*, J. Chem. Phys. **135**, 244102 (2011)

[C3.13:11] ‡ A.S.P. Gomes and Ch.R. Jacob, *Quantum-chemical embedding methods for treating local electronic excitations in complex chemical systems*, Annu. Rep. Prog. Chem. Sect. C **108**, 222 (2012)

[C3.13:12] A.J. Atkins, Ch.R. Jacob, and M. Bauer, *Probing the electronic structure of substituted ferrocenes with high resolution XANES spectroscopy,* Chem. Eur. J. **18**, 7021 (2012)

[C3.13:13] ‡ T. Weymuth, M.P. Haag, K. Kiewisch, S. Luber, S. Schenk, Ch.R. Jacob, C. Herrmann, J. Neugebauer, and M. Reiher, *MoViPac: Vibrational Spectroscopy with a Robust Meta-Program for Massively Parallel Standard and Inverse Calculations*, J. Comput. Chem. **33**, 2186 (2012)

[C3.13:14] ‡ Ch.R. Jacob and M. Reiher, *Spin in Density-Functional Theory*, Int. J. Quantum Chem. **112**, 3661 (2012)

[C3.13:15] S. Bernadotte, A.J. Atkins, and Ch.R. Jacob, *Origin-independent calculation of quadrupole intensities in X-ray absorption spectroscopy,* J. Chem. Phys. **137**, 204106 (2012)

[C3.13:16] * S. Bernadotte, F. Evers, and Ch.R. Jacob, *Plasmons in Molecules*, J. Phys. Chem. C **117**, 1863 (2013)

[C3.13:17] ‡ K. Boguslawski, Ch.R. Jacob, and M. Reiher, *Optimized Unrestricted Kohn-Sham Potentials from Ab-Initio Spin Densities*, J. Chem. Phys. **138**, 044111 (2013)

[C3.13:18] ‡ K. Kiewisch, Ch.R. Jacob, and L. Visscher, *Quantum-Chemical Electron Densities of Proteins and of Selected Protein Sites from Subsystem Density Functional Theory*, J. Chem. Theory Comput. **9**, 2425 (2013)

[C3.13:19] A.J. Atkins, M. Bauer, and Ch.R. Jacob, *The chemical sensitivity of X-ray spectroscopy: High energy resolution XANES versus X-ray emission spectroscopy of substituted ferrocenes*, Phys. Chem. Chem. Phys. **15**, 8095 (2013)

[C3.13:20] ‡ A.S.P. Gomes, Ch.R. Jacob, F. Réal, L. Visscher, and V. Vallet, *Towards systematically improvable models for actinides in condensed phase: the electronic spectrum of uranyl in $Cs_2UO_2Cl_4$ as a test case*, Phys. Chem. Chem. Phys. **15**, 15153 (2013)

[C3.13:21] Ch.R. Jacob and J. Neugebauer, *Subsystem Density-Functional Theory*, WIREs Comput. Mol. Sci. **4**, 325 (2014)

Invited Talks at International Conferences

Ch. R. Jacob, Invited lecture, Fall Meeting of the Swiss Chemical Society, Division of Computational Chemistry, Towards a subsystem density-functional theory description of covalent bonds, 16 September 2010, Zurich, Switzerland.

Ch. R. Jacob, Invited lecture, Workshop “Contacts to and Within Molecules”, Subsystem quantum chemistry for describing contacts to and within molecules, 19 September 2012, Hamburg, Germany.

Ch. R. Jacob, Invited plenary lecture, CECAM-Workshop “Vibrational Optical Activity”, 24 September 2012, Pisa, Italy.

Ch. R. Jacob, Invited Lecture, Theoretical Vibrational Spectroscopy with Localized Modes, Conference “Vibrational Dynamics”, 22 July 2013, Telluride, CO, USA.

Ch. R. Jacob, Invited Lecture, What's New in Subsystem DFT?, Workshop "DFT-based Multilayer Methods for Nanoscale System", 20 August 2013, Leiden, Netherlands.