

### 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)<sub>N</sub> and (GG)<sub>N</sub> 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  $\beta$ -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)