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DFT for isomers in solution, redox potentials, transition states and favored reaction products

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Apart from merely computationally running molecular energy optimizations and determining optimal geometries, a large variety of other techniques and applications also exist.
In this presentation uncomplicated methods are shared by which:
1. isomer geometries in solution may be determined by involving TDDFT,
2. redox potentials of series of metal complexes are determined merely from optimization HOMO & LUMO energies,
3. transition states of photo-excited species are established from energy minima on computed energy surfaces, and
4. favored complex reaction products are computed by means of reaction energy and molecular orbital calculations.

References:
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2. Redox Potentials of Ligands and Complexes – a DFT Approach, Von Eschwege, K. G.; Conradie, J., SA Journal of Chemistry, 64, 203–209, 2011, http://reference.sabinet.co.za/webx/access/electronic_journals/chem/chem_v64_a33.pdf
3. Ultrafast Photochemistry of Dithizonatophenylmercury(II), Schwoerer, H.; Von Eschwege, K. G.; Bosman, G.; Krok, P.; Conradie, J., ChemPhysChem, 2653-2658, 2011, http://onlinelibrary.wiley.com/doi/10.1002/cphc.201100337/abstract
4. Synthesis and structure of dithizonato complexes of antimony(III), copper(II) and tin(IV), Trevor T. Chiweshe, Marilé Landman, Jeanet Conradie & Karel G. von Eschwege, Journal of Coordination Chemistry, 2016, 69(5) 788–800, http://dx.doi.org/10.1080/00958972.2016.1145213

HPC content

From personal work/data, the purpose of this oral presentation is to share and instruct in an uncomplicated way, teaching 4 very handy techniques by which important chemical data and insight may be obtained computationally, in this case, DFT-B3LYP, TDDFT, etc

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