



Introduction to Machine Learning for Chemists: Visualization, Data Processing, Analysis

S. Christodoulou, N. Bernard, I. C. Gerber, F. Jolibois and R. Poteau

Python in the Physical Chemistry lab (pyPhysChem) github repository, release v. 1.9.0 (2024), doi: [10.5281/zenodo.8396813](https://doi.org/10.5281/zenodo.8396813)



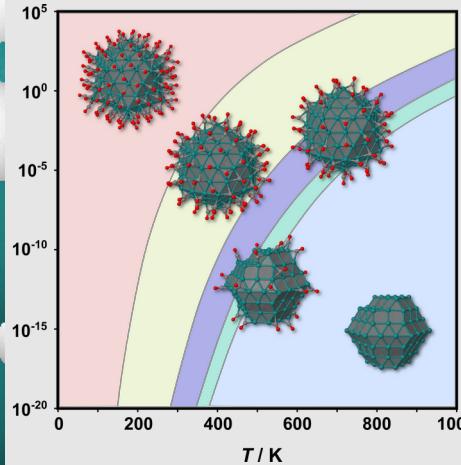
Laboratoire
de Physique & Chimie
des Nano-Objets

R. Poteau: Scientific activity in a nutshell

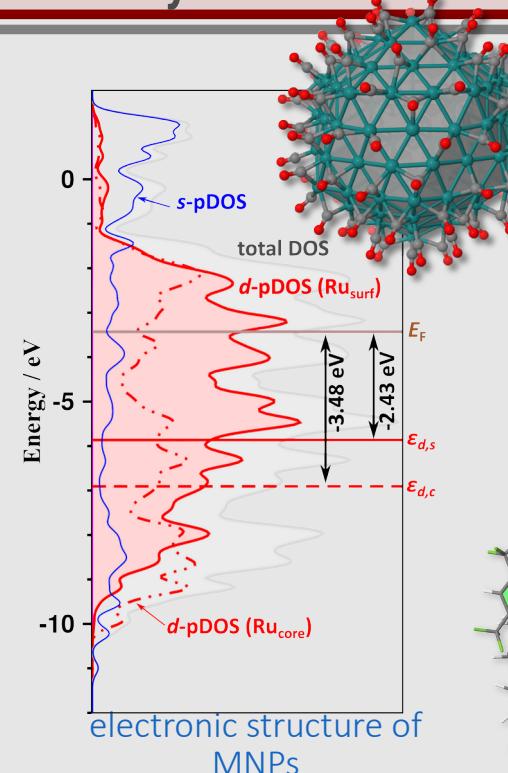
Green Chem. (2021) **23**: 8480. Link

Applied Quantum Chemistry

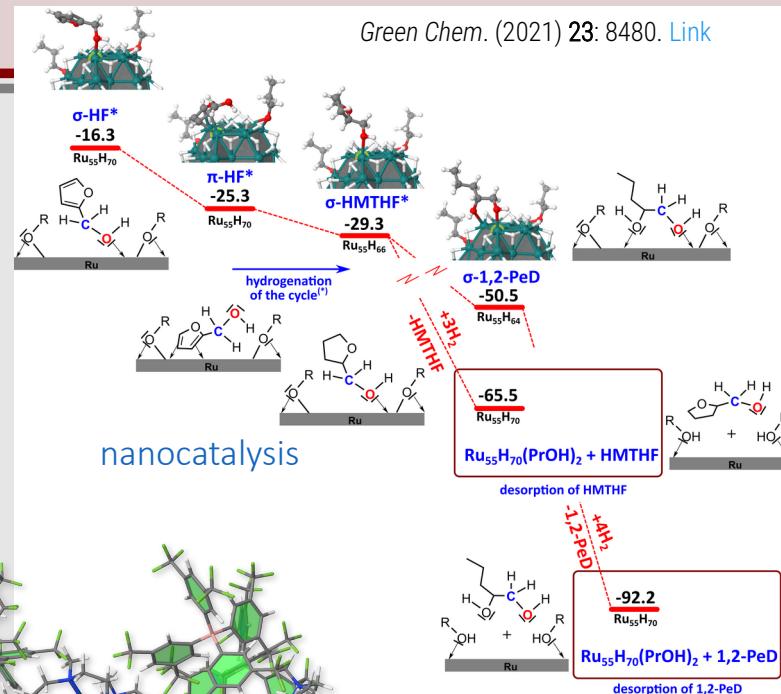
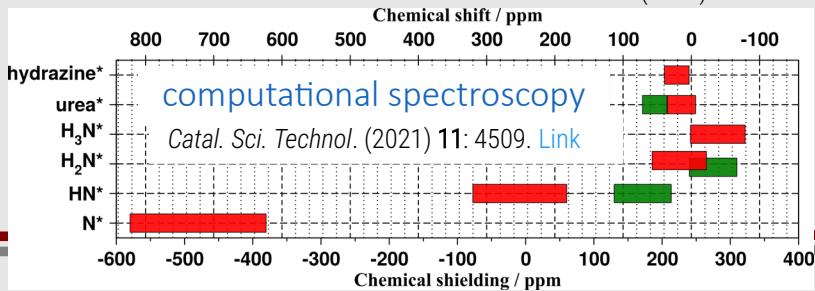
DFT (Gaussian)
DFT with PBC (VASP)
(basic tools freely available)



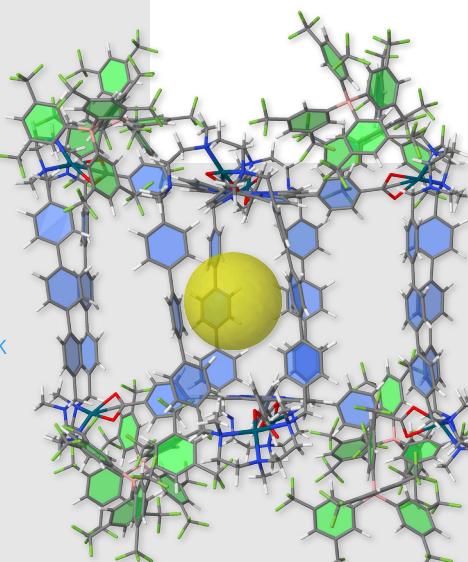
3D structure and stability of colloidal MNPs



Chem. Mater. (2022) **34**: 2931-2944. [Link](#)



Nanoscale Horiz. (2022) 7: 607. Link



“holistic” approach ← physical chemistry