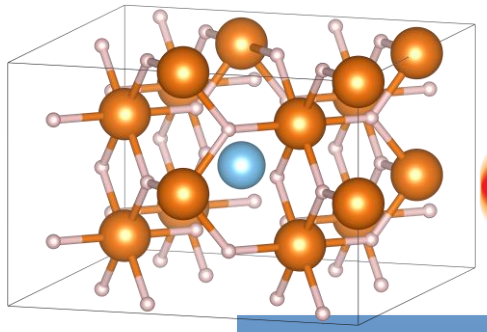
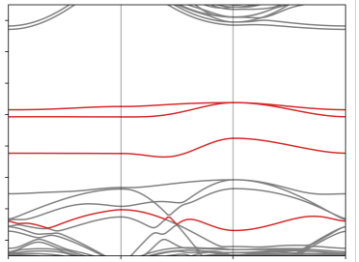
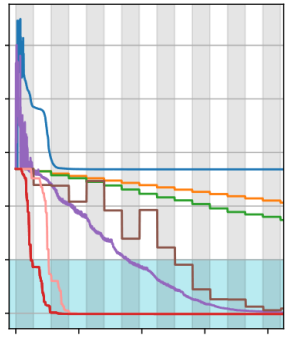
Dopyqo: Many-body analysis on top of DFT calculations

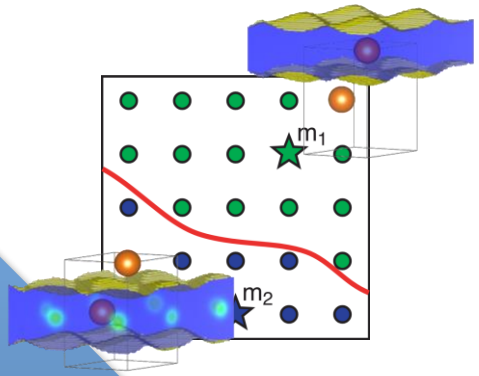




QUANTUMESPRESSO

$$\hat{H}^{(\mathbf{k})}_{\text{elec}} = \sum_{tu} h^{(\mathbf{k})}_{tu} \hat{a}^\dagger_t \hat{a}_u + \frac{1}{2} \sum_{tuvw} h^{(\mathbf{k})}_{tuvw} \hat{a}^\dagger_t \hat{a}^\dagger_u \hat{a}_v \hat{a}_w + E_{\text{n-n}} + E_{\text{e-self}}$$





Material → DFT Simulation → Many-body Hamiltonian → Ground state → Properties

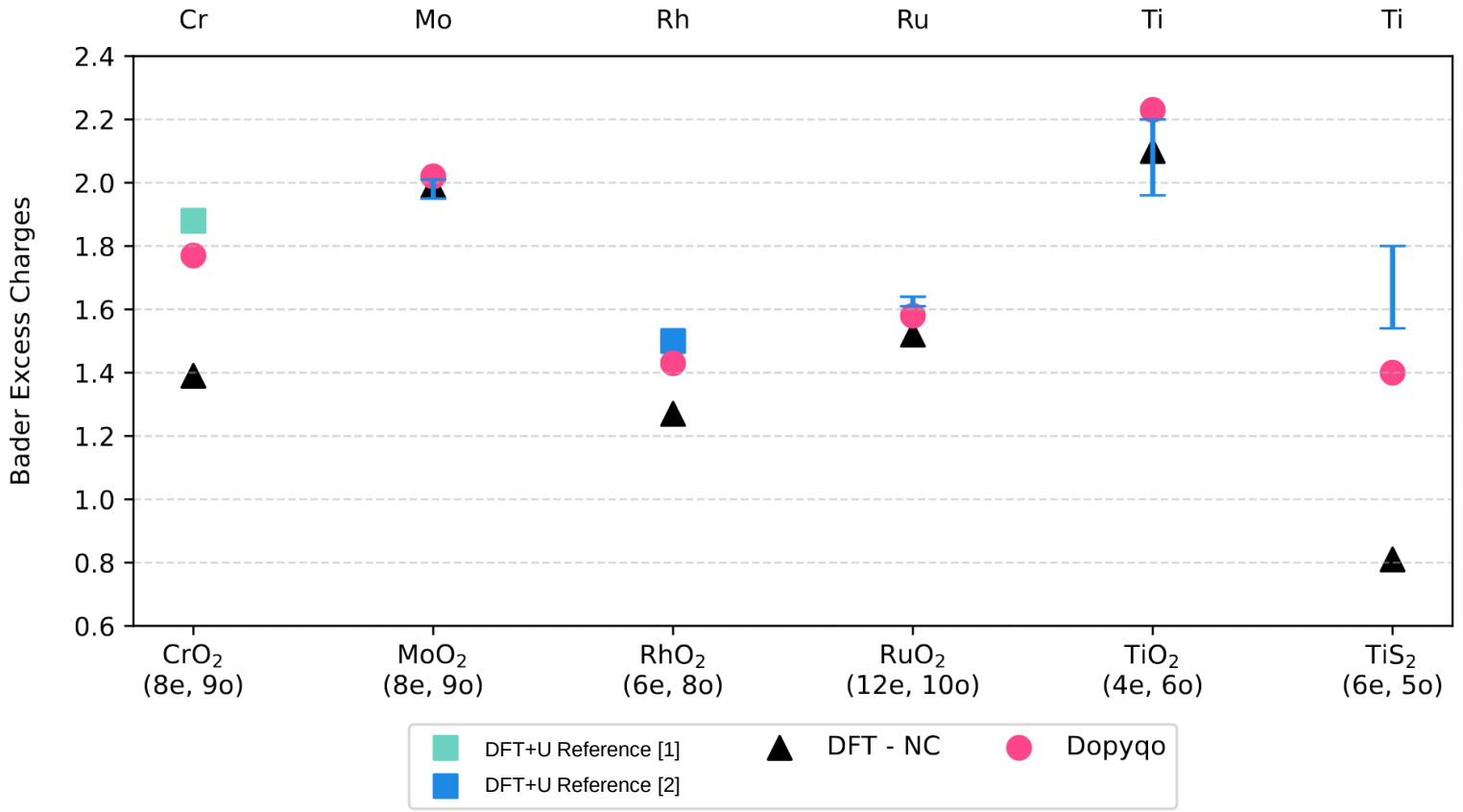
pip install dopyqo

DLR-WF/Dopyqo

Erik Schultheis, DLR Institute of Materials Research, 20.10.2025

[1] Lu et al., 2018, Phys. Rev. B
[2] Choudhuri et al., 2020, J. Chem. Theory Comput.

Use-case example: Bader charges



Use density $\rho(\boldsymbol{r}) = \sum_t f_t |\psi_t(\boldsymbol{r})|^2$ to assign each atom a

partial charge $Q_I = \int_{B_I} \rho(\boldsymbol{r})\, \mathrm{d}^3\boldsymbol{r}$ **with VQE**: $f_t^{\mathrm{VQE}} = \langle \Psi_{VQE} | \hat{n} | \Psi_{VQE} \rangle$

Improved Bader charges towards DFT+U reference

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