# Exchange–correlation functional cloning with neural networks

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Predictive accuracy in quantum materials simulations critically depends on the exchange–correlation (XC) functional within Kohn–Sham density functional theory (DFT). In Perdew's Jacob's ladder [1], approximations are organized hierarchically by their input ingredients, with higher rungs systematically improving accuracy. In practice, semi-local functionals on the GGA rung, with PBE as the most popular example, remain standard for large-scale applications due to their robustness and efficiency, but GGAs exhibit well-known limitations.

Recent advances use data-driven parameterizations, including neural networks trained on high-level wave-function data, to construct next-generation XC functionals, addressing some GGA limitations. Yet transferability, self-consistent stability, and physically consistent initialization remain central challenges.

Here, we focus on a controlled initialization setting, training a neural network to reproduce a known functional while restricting to a single rung. This allows systematic assessment of methodological choices while maintaining compatibility with standard implementations.

Networks are trained on the SLIM05 subset of GMTKN55 and evaluated on the larger SLIM16 set. Imposing physical constraints significantly improves accuracy (Fig. 1), enabling near-exact reproduction of PBE. Transferability is assessed across electronic-structure implementations (PySCF vs. SIESTA), showing networks trained only on pseudopotential densities fail to generalize to all-electron calculations, though reaction energies remain largely unaffected. Finally, insights from this controlled cloning study, particularly the benefits of physical constraints, are also seen in full training against high-level reference data.

Overall, our results provide practical guidelines for constructing and initializing self-consistent ML-XC functionals within a fixed rung of Jacob's ladder and establish a structured platform for next-generation data-driven functionals.

References

[1] Perdew J., AIP Conference Proceedings, vol 577 (2001) 1-20.
[2] Perdew J. *et al.*, Phys. Rev. Lett., 77(18) (1996) 3865–3868.
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Figures

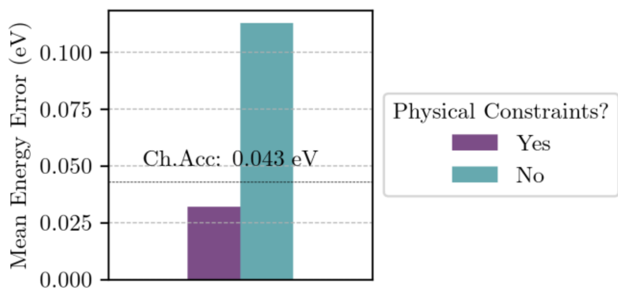


**Figure 1:** Mean energy error with respect to PBE for networks pretrained in slim05 and tested in slim16 with and without physical constraints.