Abstract Submitted
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Finding Effective Models in Transition Metals using Quantum Monte Carlo[1] KIEL WILLIAMS, LUCAS K. WAGNER, University of Illinois at Urbana-Champaign — There is a gap between high-accuracy ab-initio calculations, like those produced from Quantum Monte Carlo (QMC), and effective lattice models such as the Hubbard model. We have developed a method that combines data produced from QMC with fitting techniques taken from data science, allowing us to determine which degrees of freedom are required to connect ab-initio and model calculations[1]. We test this approach for transition metal atoms, where spectroscopic reference data exists. We report on the accuracy of several derived effective models that include different degrees of freedom, and comment on the quality of the parameter values we obtain from our fitting procedure. [1] Changlani, Zheng, and Wagner J. Chem. Phys. 143, 102814 (2015).

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