

From real materials to model Hamiltonians: multiscale modelling of strongly correlated electronic systems

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Given a realistic material with all its intrinsic complications, how does one develop simple reliable models for understanding its properties? Theoretical insight has been the key driver of this process leading to simple few-band pictures. When the interactions are comparable or much stronger than the kinetic energy, it is convenient to adopt the real space lattice approach. The effective Hamiltonian involves a considerable renormalization of parameters. Estimating these values is important for several applications in physics and chemistry. Bands/states far from the Fermi level play a significant role in the screening of Coulomb interactions leading to Hubbard U's that have been traditionally hard to determine reliably. Here we discuss an approach that we have been developing which builds in several safeguards and provides a way of obtaining effective Hamiltonians which can be simulated using techniques specifically defined for small local Hilbert spaces.

I. INTRODUCTION TO DOWNFOLDING

II. CRITERIA FOR MATCHING

III. SURVEY OF MODEL HAMILTONIANS - HUBBARD, KANAMORI,

IV. SURVEY OF DFT BASED DOWNFOLDING AND KNOWN LIMITATIONS

V. POSING THE PROBLEM/VISUALIZING THE GOODNESS OF FIT/CONNECTING TO TOOLS FROM DATA SCIENCE

VI. CHOICE OF NORM AND AVOIDING OVERFITTING: L_1 , L_2 OR SOMETHING ELSE?

VII. CHOOSING THE OPTIMAL ONE BODY SPACE/ DUAL OPTIMIZATION OF HAMILTONIAN PARAMETERS AND BASIS SETS

VIII. SIMPLE EXAMPLES - LATTICE TO LATTICE DOWNFOLDING - THREE TO ONE BAND MODEL AND THE "EFFECTIVE" D ORBITALS

IX. REALISTIC APPLICATIONS FROM ONE TO MANY BAND MODELS- SILICON, CARBON, TRANSITION METALS, TRANSITION METAL OXIDES

X. THE NEED FOR INCLUDING SPIN-ORBIT TERMS, NEED FOR QMC FOR THIS CASE

XI. PROSPECTS FOR OTHER AREAS: MAGNETISM, SMALL ENERGY SCALES

XII. APPLICATIONS TO NON QMC METHODS - COUPLED CLUSTER, FCI, HCI

XIII. STRENGTHS AND LIMITATIONS OF EFFECTIVE HAMILTONIAN APPROACH