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Advancing Efficient All-Electron Electronic Structure Methods Based on Numeric Atom-Centered Orbitals for Energy Related Materials[1]

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This talk describes recent advances of a general, efficient, accurate all-electron electronic theory approach based on numeric atom-centered orbitals; emphasis is placed on developments related to materials for energy conversion and their discovery. For total energies and electron band structures, we show that the overall accuracy is on par with the best benchmark quality codes for materials, but scalable to large system sizes (1,000s of atoms) and amenable to both periodic and non-periodic simulations. A recent localized resolution-of-identity approach for the Coulomb operator enables $O(N)$ hybrid functional based descriptions of the electronic structure of non-periodic and periodic systems, shown for supercell sizes up to 1,000 atoms; the same approach yields accurate results for many-body perturbation theory as well. For molecular systems, we also show how many-body perturbation theory for charged and neutral quasiparticle excitation energies can be efficiently yet accurately applied using basis sets of computationally manageable size. Finally, the talk highlights applications to the electronic structure of hybrid organic-inorganic perovskite materials, as well as to graphene-based substrates for possible future transition metal compound based electrocatalyst materials.

[1]All methods described here are part of the FHI-aims code. VB gratefully acknowledges contributions by numerous collaborators at Duke University, Fritz Haber Institute Berlin, TU Munich, USTC Hefei, Aalto University, and many others around the globe.