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Title: Pushing some computational limits with all-electron electronic structure theory: Eigenvalue solvers, surface reconstruction, biomolecular structure

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Electronic structure theory is the workhorse of computational materials science today, promising an essentially standalone, parameter-free description of materials, (bio)molecules, chemical reactions etc. Among the primary challenges are sufficiently accurate exchange-correlation treatments that are feasible for the necessary system sizes, time scales, and possibly statistical averages. To meet these challenges, it is essential to use today's computational resources (including massively parallel architectures) effectively. On the application side, this contribution focuses on an accurate description of large-scale reconstructed surfaces, as well as the complex conformational energy landscapes of biomolecular systems (here, polyalanine-based peptides). Reconstructed surfaces necessitate an accurate treatment of potentially thousands of heavy atoms, whereas in the biomolecular case, an enormously large conformational space is distinguished by rather subtle interaction terms (hydrogen bonds, van der Waals), and finite-temperature effects can not be neglected. We address these challenges within our all-electron electronic structure code FHI-aims (http://aims.fhi-berlin.mpg.de/). Based on numeric atom-centered orbitals, the code enables efficient, accurate treatments of molecular and solid systems using standard density-functional theory (LDA and GGA), as well as hybrid functionals and (for non-periodic systems) many-body approaches such as RPA or GW. We address some important computational prerequisites for massively parallel scalability, in particular the generally applicable, conventional eigenvalue solver ``ELPA" (http://elpa.rzg.mpg.de) which significantly pushes out the scalability of the Kohn-Sham generalized eigenvalue problem on high-performance computing platforms (Intel/Infiniband, BlueGene/P, Cray).