State of FHI-aims

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This presentation focuses on the Fritz Haber Institute *ab initio* molecular simulations package, our implementation of "density functional theory and beyond" for molecules and materials based on numeric atom-centered orbitals. Over a period of eight years, the code has become a solid, capable framework for reliable production electronic structure theory (density functional based total energy and force methods for non-periodic molecular systems and periodic solids) and for many individual developments that build on this foundation. Recent additions cover areas as diverse as periodic hybrid functionals for solids, self-consistent *GW* and methods "beyond RPA or *GW*" for molecules, a full molecular transport framework, path integral molecular dynamics, (finally) an analytic version of the stress tensor for solids, and a host of other improvements, many of which will be discussed in depth at the workshop. In my talk, I will attempt an overview of past progress and future challenges, including some examples of large-scale applications of the code. As a whole, FHI-aims is the product of an active network of contributors both in Berlin and around the globe. This talk is dedicated to their efforts.