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Enhancing Linear-Scaling DFT for Extended Systems via a QM/QM Fragment Approach LAURA RATCLIFF, Argonne National Laboratory, LUIGI GENOVESE, CEA Grenoble, STEPHAN MOHR, Barcelona Supercomputing Center, THIERRY DEUTSCH, CEA Grenoble — We recently introduced a minimal basis approach to the wavelet-based BigDFT code, wherein a minimal set of localized support functions are expressed in an underlying wavelet basis and optimized to reflect their chemical environment. This not only forms the basis of an accurate linear-scaling DFT approach, allowing systems of 10,000 atoms or more to be treated with modest computational resources, but also facilitates the straightforward definition of a fragment approach. Such an approach can reduce the computational cost by an order of magnitude while also offering additional flexibility. We have previously demonstrated the suitability of a molecular fragment approach for the treatment of environmental effects within the context of constrained DFT and have now also expanded the method to include the treatment of extended, periodic systems. In this talk we will describe the extended fragment approach and present examples of its application to large defect systems, as well as offering a perspective on future directions for the treatment of very large systems, such as an embedded approach.

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