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Local atomic energies from optimal atomic orbitals BJÖRN LANGE, CHRISTOPH FREYSOLDT, JÖRG NEUGEBAUER, Max Planck Institute for Iron Research GmbH — Decomposing the energy of a condensed matter system into atomic contributions is of great use e.g. for understanding the physical origin of defect and surface energetics or for identifying chemically reactive regions in disordered systems. However, commonly employed energy calculations in the framework of density-functional theory (DFT) do not in general provide a natural decomposition into atoms. Here we propose a novel scheme to achieve this based on the recently introduced concept of atom-centered Quamols [1] that are variationally optimized to represent the electronic structure with a minimal basis set, which largely avoids local overcompleteness issues. The spillage resulting from the remaining small incompleteness is segmented according to a space separation derived from the Quamol atomic densities, maintaining the accuracy of the underlying DFT calculation. The total energy is then decomposed by combining this basis set with a local energy density treatment based on the ideas of Chetty and Martin [2]. We demonstrate the performance of our scheme by visualizing and analyzing the energy distribution at surfaces and in amorphous silicon.

[1] Lange, B et al., Phys. Rev. B 84, 085101, (2011)
[2] Chetty, N. and Martin, Richard M., Phys. Rev. B 45, 6074, (1992)

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