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Prediction of a reconstructed α-boron (111) surface by the minima hopping method MAXIMILIAN AMSLER, STEFAN GOEDECKER, University of Basel, SILVANA BOTTI, MIGUEL A.L. MARQUES, Université Lyon 1-CNRS — Boron exhibits an impressive structural variety and immense efforts have recently been made to explore boron structures of low dimensionality, such as boron fullerenes, two-dimensional boron sheets or boron nanotubes which are theoretically predicted to exhibit superior electronic properties compared to their carbon analogues. By performing an extensive and systematic *ab initio* structural search for the (111) surface of α-boron (111) using the minima hopping structure prediction method we found very strong reconstructions that lead to two-dimensional surface layers. The topmost layer of these low energy reconstructions is a conductive, nearly perfectly planar boron sheet. If exfoliation was experimentally possible, promising precursors for a large variety of boron nano-structures such as single walled boron nanotubes and boron fullerenes could be obtained.

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