Abstract Submitted
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Large-scale surface reconstructions from first principles: Au(100) and Pt(100) by all-electron DFT PAULA HAVU, VOLKER BLUM, VILLE HAVU, PATRICK RINKE, MATTHIAS SCHEFFLER, Fritz Haber Institute, D-14195 Berlin, Germany — We show that the large-scale, quasihexagonal surface reconstructions of Au(100) and Pt(100) are captured by all-electron density functional theory (DFT) in the local-density approximation and PBE generalized gradient approximation in excellent agreement with experiment. While the superstructure is often approximated as (5×1) in first-principles calculations, larger, more realistic approximants turn out to be important for some aspects. For example, the reconstruction energy for Au(100) approximately doubles compared to (5×1) when considering the much larger, more realistic series (5×N) (N=10,15,20,25,30). For Pt(100), where an experimental reconstruction energy estimate exists [1], DFT based on these approximants is in close agreement. In addition to the energetics, our calculations reveal the full local surface geometry, and corroborrate relativistically enhanced *d*-*d* hybridization as the electronic reconstruction driving force. Our calculations are based on 5-layer asymmetric slab geometries, two layers of which are fully relaxed, i.e. up to 786 atoms, with 336 relaxed, and are performed using the efficient, accurate all-electron electronic structure code FHI-aims [2]. [1] W.A. Brown, R. Kose, D.A. King, Chem. Rev. **98**, 797 (1998) [2] V. Blum *et al*, Comp. Phys. Comm. **180**, 2175 (2009).

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