Abstract Submitted
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Investigation of the liquid Pb/Si(001) interface from ab initio molecular-dynamics calculations[1] D.J. GONZALEZ, Universidad de Valladolid, Spain, J. SOUTO, M.M.G. ALEMANY, R.C. LONGO, L.J. GALLEGO, Universidad de Santiago de Compostela, Spain, L.E. GONZALEZ, Universidad de Valladolid, Spain — The structure of liquid Pb on an ideal Si(001) surface was studied experimentally a decade ago by means of x-ray diffraction and the results were interpreted in terms of the presence of fivefold symmetry Pb structures captured transiently by the potential created by the unreconstructed Si(001) surface. We critically analyze this interpretation in the light of the results obtained in an extensive ab initio molecular dynamics study of a system comprising 314 Pb atoms and 175 Si atoms setup in 7 (001) ideal layers (a total number of 1956 valence electrons) in a slab geometry. The structure found for the first Pb layer is very different from that of bulk Pb, mostly consisting in one-dimensional lines. However, we do observe the possibility of forming transient structures, in particular icosahedral caps.

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