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Ab-Initio Studies of Properties of 2D Rare-Earth Silicide Surfaces CHRISTOPHER EAMES, STEVE TEAR, MATTHEW PROBERT, Dept of Physics, University of York, UK — Rare Earth overlayers on the Si(111) surface have attracted interest due to their novel properties [1,2] and the unusual reconstruction that is formed with a flat rare earth layer buried inside the Silicon [3,4,5,6]. Here we present the results of ab-initio calculations done using the CASTEP [7] code to determine the structural and electronic properties of these reconstructions. We compare these to those derived experimentally.

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