

Abstract Submitted
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LEED and Ab-Initio Study of the SmSi(111)-3x2 Reconstruction CHRISTOPHER EAMES, STEVE TEAR, MATTHEW PROBERT, Dept of Physics, University of York, UK — The Si(111)3x2-Sm reconstruction that has been observed by STM produces a 3x1 pattern when viewed using LEED [1]. It has been suggested that similar behaviour for Si(111)3x2-Ba is due to the interference of the emergent electron amplitudes between adjacent registry shifted unit cells [2]. We have gathered LEED I(V) curves from this surface and here we present a quantitative comparison of these with a structural model that has been suggested in the literature [3] and with the results of our own ab-initio calculations done using the CASTEP [4] code.

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- [2] J. Schafer *et al*, *Phys. Rev. B.*, **67** (2003) 85411-85415
- [3] E. Ehret *et al*, *Surf. Sci.*, **569** (2004) 23-32
- [4] M. D. Segall *et al*, *J. Phys.: Cond. Matt.*, **14** (2002) 2717-2743

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