

Abstract Submitted
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Detailed Structure Determination of Nanostructures by Low-Energy Electron Diffraction.¹ MICHEL VAN HOVE, G.M. GAVAZA, Z.X. YU, City University of Hong Kong, L. TSANG, University of Washington-Seattle, C.H. CHAN, S.Y. TONG, City University of Hong Kong — Detailed structural information of nanostructures (e.g. bond lengths and bond angles) is needed to allow the understanding and prediction of their physical and other properties. To that end we have extended the theoretical capabilities of surface structure determination by Low Energy Electron Diffraction (LEED) to nanostructures. Our new computational method has a compute time that scales as $N \log N$ in terms of the number N of independent atoms, in contrast to N^2 or N^3 which typical of conventional LEED calculations of electron multiple scattering. We exhibit the resulting ability to solve detailed nanostructures of different kinds: buckyballs adsorbed on a Cu(111) surface; endohedral and exohedral buckyballs with additional Li or Cu atoms; adsorbed carbon nanotubes; and silicon nanowires. This demonstration of the capability to solve nanostructures should spur the development of experimental methods to measure electron diffraction from nanostructures.

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Michel Van Hove
City University of Hong Kong

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