

Abstract Submitted
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Determination of Adsorbed C₆₀ Nanostructures by Low-Energy Electron Diffraction¹ M.A. VAN HOVE, G.M. GAVAZA, Z.X. YU, G. XU, S.Y. TONG, City University of Hong Kong, W.W. PAI, C.H. LIN, Center for Condensed Matter Sciences, National Taiwan University — We have recently extended to nanostructures the basic theoretical capabilities of surface structure determination by Low Energy Electron Diffraction (LEED), by adopting a non-periodic cluster approach and substantially accelerating the computation time for complex structures. In this contribution, we describe two further theoretical enhancements and their application to experimental data for buckyballs adsorbed on a Cu(111) surface. One enhancement addresses occasional situations where strong multiple scattering causes poor convergence: this is solved by treating all scattering within subclusters of a few atoms with accurate matrix inversion. Secondly, for the structure determination of complex nanostructures, an efficient search method is essential: for that purpose a modified version of tensor LEED is adapted to nanostructures, called NanoTensor-LEED. We exhibit the resulting ability to analyze detailed nanostructures with the case of buckyballs adsorbed on a Cu(111) surface.

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M.A. Van Hove
City University of Hong Kong

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