

## AN APPLICATION OF CLASSICAL MOLECULAR DYNAMICS SIMULATION AND AB INITIO DENSITY-FUNCTIONAL CALCULATION IN SURFACE PHYSICS

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Classical molecular dynamics simulation and ab initio mixed basis Car-Parrinello methods are discussed and applied to the investigation of the results of a recently performed STM based experiment involving the adsorption of  $C_{60}$  molecules on the disordered Si surface. We show that these methods are capable of providing the theoretical basis for this experiment and for the validity of the associated conclusions.

A mixed-basis self-consistent formalism for the Car-Parrinello method is proposed to obtain the detailed understanding of the electronic states and dynamics of surface stresses. A band structure calculation using this formalism is performed for the  $c(2 \times 2)$  structure of  $C_{60}$  adsorbed on Si (100) surface and is compared with the experimental results.

**KEY WORDS:** Classical MD simulation, Car-Parrinello method, mixed-basis DFT,  $C_{60}$  molecules, Si(100)  $c(2 \times 2)$  surface, Tersoff potential

### 1. INTRODUCTION

Computer-based Molecular Dynamics (MD) simulations have now become standard methodologies for investigating, at the atomistic and molecular levels, theoretical and experimental problems in condensed matter physics and materials science. Employing these methods, we are now able to understand the collective behaviour and properties of complex systems and their emergent properties in condensed phase in terms of motions of their individual constituents, and to predict their time evolutions under controlled conditions. In materials science, MD simulations have been employed over the past few years to provide insights into the processes that emerge in stressed nano volumes of solids in order to elucidate the atomistic mechanisms underlying the macroscopic processes of plastic flow, adhesion, sintering, indentation, fracture, friction and dislocation nucleation in metals [1, 2, 3].

Recently, problems in surface physics of metals and semi-conductors have provided the fertile grounds for further applications of MD simulations in materials science. The adsorptions of monolayers and multilayers of molecules and micro- and nano-clusters on metallic and semi-conducting surfaces can now be simulated to provide insights into the corresponding STM-based, and other, experimental investigations performed in this field.

A classical MD simulation proceeds by considering a finite nano-size cluster of

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