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Graphene synthesis, carbon foams, pillared graphene, pseudospheres and all that from first-principles, multiscale simulations and experiments

In this talk I will first discuss the processes leading to the room-temperature growth of carbon-based materials, notably silicon carbide (SiC) 1,2] and graphene [3,4] by supersonic molecular beam epitaxy. In particular, I will present both experiments and computational modelling of fullerene impacts on silicon and copper surfaces at intermediate-energy regimes (few tens of eV) as a novel approach to synthesise crystalline and layered materials. This collision induces strong chemical-physical perturbations in the system and, for sufficient C_{60} translational energy, disruption of molecular bonds and cage breaking. Characterization of the epitaxial grown materials by a variety of experimental techniques, such as XPS, UPS, Auger, LEED, TEM, and Raman after the collision, demonstrates the potentiality of our approach to grow nanostructured and bi-dimensional materials even at room temperature. On the theoretical side, we show that in these out-of-equilibrium conditions, it is necessary to go beyond the standard implementation of ab-initio molecular dynamics based on the Born-Oppenheimer approximation, which fails to capture the excited-state dynamics. In particular, we analyse the Si- and Cu-C_{60} collision within the non-adiabatic nuclear dynamics framework, where stochastic hops occur between adiabatic surfaces calculated via time-dependent density functional theory. The theoretical description of C_{60} impacts on metallic and semiconductor substrates will be further analysed by multiscale techniques based on Kinetic Monte Carlo and metadynamics. Finally, the application of molecular dynamics, classical minimization and Monte Carlo techniques will be shown to investigate the mechanical properties of carbon-based 3D nano-foams [5], the discovery of novel energetically stable carbon structures shaped as Beltrami pseudospheres [6], the gas-sieving properties of pillared graphene oxides (PGO) and foams [7] as well as the dielectric and charge transport properties of carbon materials [8].

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Figures

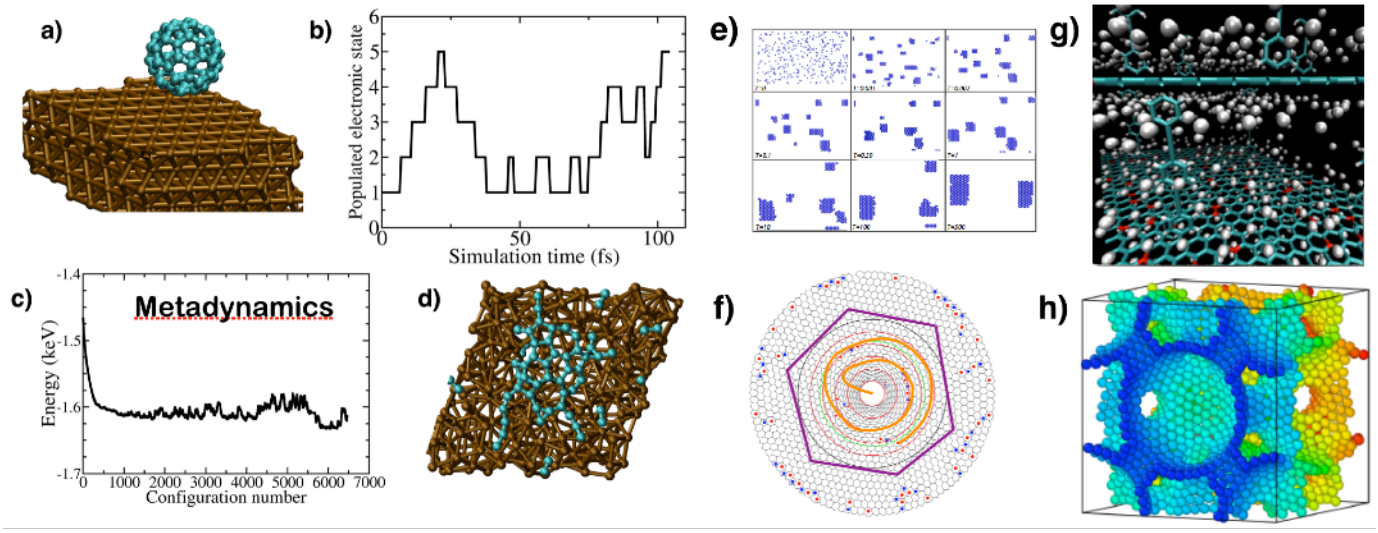

Figure 1: a) SuMBE layout, b) Non-adiabatic, c) Metadynamics, d) Graphene growts, e) Kinetic Monte Carlo, f) Graphene trumpets, g) PGO, h) Graphene 3D foams