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Numerical studies from quantum to macroscopic scales of carbon nanoparticules in hydrogen plasma GUILLAUME LOMBARDI, CNRS LSPM - University Paris 13, ALAIN NGANDJONG, ITODYS - University Paris Diderot, ZSOLT MEZEI, JONATHAN MOUGENOT, ARMELLE MICHAU, KHALED HASSOUNI, CNRS LSPM - University Paris 13, MAHAMADOU SEYDOU, FRANOIS MAUREL, ITODYS - University Paris Diderot — Dusty plasmas take part in large scientific domains from Universe Science to nanomaterial synthesis processes. They are often generated by growth from molecular precursor. This growth leads to the formation of larger clusters which induce solid germs nucleation. Particle formed are described by an aerosol dynamic taking into account coagulation, molecular deposition and transport processes. These processes are controlled by the elementary particle. So there is a strong coupling between particle dynamics and plasma discharge equilibrium. This study is focused on the development of a multiscale physic and numeric model of hydrogen plasmas and carbon particles around three essential coupled axes to describe the various physical phenomena: (i) Macro/mesoscopic fluid modeling describing in an auto-coherent way, characteristics of the plasma, molecular clusters and aerosol behavior; (ii) the classic molecular dynamics offering a description to the scale molecular of the chains of chemical reactions and the phenomena of aggregation; (iii) the quantum chemistry to establish the activation barriers of the different processes driving the nanopoarticule formation.

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