Structure and Reactivity of Interstellar Nanodust

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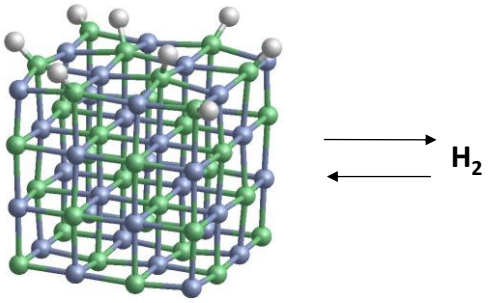
Dust plays a crucial role in the chemical evolution of the interstellar medium by catalyzing molecule formation and, through scattering strong interstellar radiation, preventing molecular photodissociation in denser regions. Via lab characterization of pristine material and astronomical observations, the general properties of dust particles in various environments have been reasonably well discerned. Fitting the observed infrared (IR) spectra with a combination of laboratory spectra of materials of different crystallinity, shape, size and composition has given valuable insight into the possible identity of dust particles in space.

We present a complementary approach to understanding the formation, structure and reactivity of small dust grains based on a bottom-up (i.e. from an atomistic and electronic level) computational modelling [1]. Crucially, our approach is independent of assumptions based on bulk materials properties, is not limited to any particular chemistry or specific thermodynamic conditions, and provides a solid basis for subsequent kinetic modelling for longer timescales associated with larger dust particle species. We specifically focus on nanoscale dust grains which are thought to form a substantial proportion of the total interstellar dust grain population and are have likely to a disproportionally high impact on astrochemistry due to their very high surface area to bulk ratios.

We consider both silicate and TiC nanodust and show how our approach can provide detailed insights into the reactivity of these species with respect to their role as ice condensation nuclei [2] and their role in H_2 formation and dissociation [3-5]. We also report accurately computed IR spectra of our considered nanodust species with relation to experimental and observed IR spectra.



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