A Bottom-up Computional Modelling Approach to the Formation and Properties Silicate Dust

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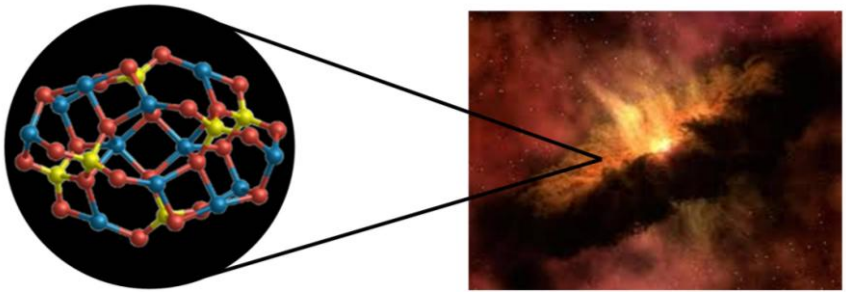
While dust takes up only one mass percent of the total matter in the interstellar medium (ISM), it plays a crucial role in its chemical evolution by catalyzing molecule formation and, through scattering the strong interstellar radiation, preventing molecular photodissociation in denser regions. Via a combination of lab characterization of pristine material, astronomical observations, the general properties of dust particles in various environments have been reasonably well discerned. Fitting the observed spectra with a combination of lab spectra of materials of different crystallinity, shape, size and composition gives valuable insight into the possible identity of dust particles in space.

We present a complementary approach to understanding the formation, structure and properties of small dust grains based on a bottom-up (i.e. starting from the atomistic and electronic level) computational modelling. Crucially, our approach is independent of assumptions based on bulk materials properties (as is the case for classical nucleation theory), is not limited to particular chemistry or specific thermodynamic conditions, and provides a solid basis for subsequent kinetic modelling for longer timescales associated with larger dust particle species.

Specifically we outline our approach for the example cases of (i) the initial stages silicate dust formation based on combining SiO, Mg, H_2O (and TiO_2) monomeric species [1,2], and the reactivity of ultra small dust grains (nanosilicates) with respect to H_2 formation and dissociation [3] and their role as ice condensation nuclei [4]. The thermal stability and IR vibrational spectra of nanosilicate dust precursors is also examined using the same modelling methods.



[1] *Efficient nucleation of stardust silicates via heteromolecular homogeneous condensation*, T. P. M. Goumans and S. T. Bromley, ***MNRAS*** 420, 3344 (2012)
[2] *Stardust silicate nucleation kick-started by SiO+TiO_2*, T. P. M. Goumans and S. T. Bromley, ***Phil. Trans. R Soc. A*** 371, 20110580 (2013).
[3] *Hydrogen and oxygen adsorption on a nanosilicate – a quantum chemical study*, T. P. M. Goumans and S. T. Bromley, ***MNRAS***, 414, 1285 (2011).
[4] *Competing mechanisms of catalytic H_2 formation and dissociation on ultrasmall silicate nanocluster dust grains*, B. Kerkeni, S. T. Bromley, ***MNRAS***, 435, 1486 (2013)