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Realistic modelling of nano-aggregated magnesium silicate dust particles using atomistic simulations.

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Dust can be found everywhere in the universe from stars in the latest stages of evolution (post-AGB stars), to the interstellar medium (ISM) and protoplanetary disks around young stars (e.g. T Tauri and Herbig Ae/Be stars). Dust can provide a wealth of information about the medium it is embedded in, since processing will affect its composition, structure and size in a characteristic and distinct manner. The properties of dust can thus also be used to track the nature of its environment. For instance, the growth of dust particles in protoplanetary disks is linked to the evolution from flared to flattered disks, while the small crystalline fraction of silicates in the ISM indicates a high degree of energetic processing.

The source of data to understand dust formation, growth, composition and shape of the dust particles is infrared (IR) spectroscopy. Nevertheless, the information provided by IR spectroscopy from laboratory synthesized particles is not well understood, due to the difficulties to control and understand the generated particles at the nanoscale level. Knowledge at the nanoscale, such as cation mobility and disorder, can be helpful in order to understand properties of silicate materials such as the crystallization below the glass transition temperature.

Bottom-up atomistic computational modelling methods allow the study of particles with atomic-scale precision, but in order to perform such simulations we require realistic models of the particles of interest. Here we present an new approach that uses well-tailored interatomic potentials to simulate the growth of silicate nanoparticles with diameters up to of tens nanometres following the detailed circumstellar nucleation conditions typical for a post-AGB star. The simulations progressively and realistically add monomers (SiO, Mg and O) to a seed particle moving away from the star with a determined initial velocity.

We solve the equation of movement for the seed particle, and thus estimate how the typical circumstellar conditions for nucleation (e.g. temperature, pressure) change with time and thus distance from the star. From the generated atomistically detailed nanodust particle models, we can probe properties that are difficult to accurately extract from experiments such as surface structure, surface to volume ratios, degree of polymerization of silicate tetrahedra, nanoporosity and nanosized phase separation. Via analysing the vibrational atomic motions within the generated nanodust silicate particles we can also directly simulate the IR emission from such species. In this way we are able show how the IR spectra of silicate nanodust relates to changes in atomic disorder/crystallinity, chemical composition (e.g. pyroxene vs olivine) and nucleation conditions (e.g. temperature).

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