A Computational View on Astronomical Silicate Nanoclusters.

Antoni Macià Escatllar[1], Stefan T. Bromley[1,2]

1. Computational Material Science Laboratory, Departament de Ciència de Materials i Química Física and Institut de Química Teòrica i Modelització Computacional (IQTC), UB
2. Institució Catalana de Recerca i Estudis Avançats (ICREA))

Although silicates dust grains are known to be present in almost all astronomical environments, there are several open questions regarding their structure, composition and properties. Silicate dust particles form by nucleation in the circumstellar shells of Asymptotic Giant Branch (AGB) stars and gradually grow larger as they are expelled by stellar radiation pressure towards the Interstellar Medium (ISM).[1] The population of ultrasmall silicates (nanoparticles which contains few hundreds of atoms) is estimated to contain around 10% of the total mass of Si in the interstellar medium (ISM)[2] and thus, by number, are one of the most abundant dust species. Understanding the properties of such nanoclusters can help understand the conditions and processes occurring at different phases of the ISM.

Computational chemistry can provide new insights into the physical and chemical properties of this family of nanomaterials where no experimental values are available. In this talk, I'll discuss about our recent advances in modelling such nanoclusters. More specifically, we have performed an extensive global optimization searches using a newly derived interatomic potential. Subsequently, we have employed density functional theory based calculations to obtain reliable structures and energies for nanosilicates with the most common olivine (Mg_2SiO_4) and pyroxene ($MgSiO_3$) stoichiometries. In this study we have identified the presence of a highly stable pyroxene magic nanocluster which should be largely abundant in circumstellar environments, if dominated by thermodynamic conditions. We also confirm that nanosilicates of both stoichiometries have large dipole moments, in line with the required values to explain an as-yet unassigned significant component of the astronomically observed microwave spectrum – the so-called anomalous microwave emission.[3]

1. H. Gail, E. Sedlmay, Physics and Chemistry of Circumstellar Dust shells, *Cambridge University Press* (2013)
2. A. Li, B. Draine, *ApJ*. **550** L213–L217 (2001).
3. B. Hensley, B. Draine, *ApJ*, **836**, 179-183 (2017)