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The role of alumina in triggering stellar outflows

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An important dust component in Asymptotic Giant Branch (AGB) stars is aluminum oxide or alumina (stoichiometric formula Al_2O_3) showing a spectral emission feature around ∼13 μm attributed to Al−O streching and bending modes (Posch *et al.* 1999; Sloan *et al.* 2003). Alumina presolar grains are also found in pristine meteorites with typical sizes of a few tens of nm to μms (Stroud *et al.* 2004). Owing to their refractory nature (thermal stability) and the large abundances of Al- and O-bearing compounds, alumina grains are thought to represent the first condensates to emerge in the atmospheres of oxygen-rich AGB stars. In the bulk phase, alumina exists predominantly in two crystalline forms (corundum and clay). The properties of nanoparticles with sizes below ∼50 nm, however, differ significantly from bulk properties. Quantum and surface effects of these small particles lead to non- crystalline structures, whose characteristics (geometry, coordination, density, energy) may differ by orders of magnitude, compared to the bulk material. A top-down approach, like classical nucleation theory, is thus not applicable. Therefore, we follow a bottom-up approach, starting with molecular precursors (AlO, AlOH) and the smallest stoichiometric clusters (Al_2O_3, Al_4O_6). Then, we successively build up larger-sized clusters.

We present the results of the quantum-mechanical structure calculations of $(Al_2O_3)_n$ clusters with n =1−10, including potential energies, rotational constants, charge distributions and structure-specific infrared spectra (vibrational frequencies and intensities). We find new global minima candidates for cluster sizes n =8, 9, and 10, that are partly reported in Gobrecht *et al.* (2018). A homogeneous nucleation, where Al_2O_3 monomers are successively added, is energetically viable in circumstellar conditions (p =10^{-5}−10 Pa, T =500−6000 K). However, the formation of the monomer itself represents an energetic bottleneck. Moreover, the most stable monomer structure is a triplet state and has a spin barrier. A potential loophole are formation routes towards the dimer (Al_4O_6) without requiring the monomer as intermediary and pathways involving SiO as a catalyst.

The most intense vibrations of the small alumina clusters occur around 10-11 μm. Around 13 μm the overall IR intensity is rather low. Also other characteristics (energy, coordination, bond lengths) indicate that the bulk limit is not reached for $(Al_2O_3)_n$ clusters, n =1−10, with a size range of d≤1 nm.

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