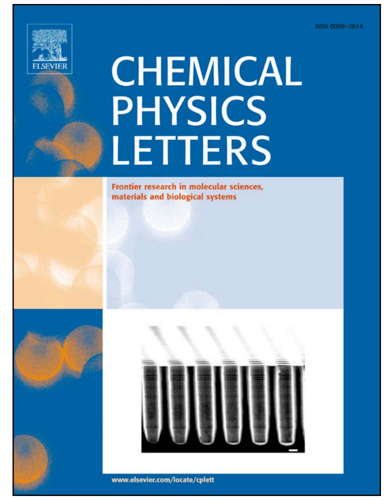

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A global optimisation study of the low-lying isomers of the alumina octomer $(Al_2O_3)_8$

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Abstract

We employ the Monte-Carlo Basin-Hopping (MC-BH) global optimisation technique with inter- atomic pair potentials to generate low-energy candidates of stoichiometric alumina octomers ($(Al_2O_3)_8$). The candidate structures are subsequently refined with density functional theory calculations employing hybrid functionals (B3LYP and PBE0) and a large basis set (6-311+G(d)) including a vibrational analysis. We report the discovery of a set of energetically low-lying alumina octomer clusters, including a new global minimum candidate, with shapes that are elongated rather than spherical. **We find a stability limit for these and smaller-sized clusters at a temperature of $T \simeq 1300 - 1450$ K corresponding to a phase transition in liquid alumina.**

Keywords: aluminum oxide, molecular clusters, global optimisation, nucleation

1. Introduction

Alumina clusters play a role in atmospheric chemistry [1]. Being artificially produced by rocket flights, Al_2O_3 cluster aerosols impact the Earth's atmospheric chemistry as they act as catalysts. Moreover, owing to their high thermal stabilities and (near)-infrared properties, alumina clusters are promising candidates to form the seed nuclei of dust formation in oxygen-rich AGB stars [2, 3, 4, 5]. Although silicate dust constitutes the major part of oxygen-rich cosmic dust, its nucleation solely from gas-phase precursors is energetically hampered and explicitely ruled out for SiO [6, 7] and MgO [8, 9]. Instead, it is more likely that the silicate dust forms on top of pre-existing seed nuclei. These seed nuclei must form from available atoms and molecules, and have to sustain the extreme thermodynamic conditions close to the stellar surface. In oxygen- dominated regimes, the latter requirement are fulfilled by highly refractory metal oxides such as alumina (Al_2O_3) and titania (TiO_2). Studies on stardust grains from pristine meteorites show

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