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Evidence of pyroxene magic nanoclusters in protoplanetary disks around Herbig Ae stars from first principles calculations

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From infrared (IR) observations it is known that magnesium silicates are the major dust component in protoplanetary disks. From such observations one can discern the likely size, composition and crystallinity of such dust thus allowing one to infer the likely associated properties of the disk. Of special interest are the disks surrounding Herbig Ae/Be (HAeBe) stars corresponding to the stellar evolutionary stage where embryonic planets should be forming.

Using Spitzer IR data, Juhasz et al. [1] derived the averaged mass absorption coefficient (MAC) of the crystalline pyroxene component from a selected set of HAeBe stars and compared it with experimentally derived MACs of different bulk crystalline pyroxene samples. The star-derived MAC was found to contain signals in regions that do not appear in the experimental crystalline pyroxene MACs (e.g. a sharp feature at 8.7 microns and a broad region between 14.4 - 16.4 microns). Using accurate first principle electronic structure calculations, we provide evidence that the spectral mismatches between experimental and observationally derived MACs for crystalline pyroxene could be explained by the presence of pyroxene nanodust.

Using dedicated global optimisation search algorithms we have established the most stable atomic scale structures of a range of pyroxene nanoclusters (MgSiO3)N for N = 1 - 10. Within this set we identified those clusters with particularly high energetic stability with respect to other clusters of a similar size. Such so-called "magic"clusters are known from cluster beam experiments to have disproportionally high abundances in cluster populations. Correspondingly, one should expect that, if nano-pyroxene dust forms a reasonable proportion of the pyroxene silicate dust budget in protoplanetary disks, then magic pyroxene clusters may be particularly abundant. We found that the pyroxene nanosilicate cluster (MgSiO3)5 was indeed a magic cluster and thus a possible abundant dust candidate. Using first principles density functional theory (DFT) based electronic structure calculations we then calculated the accurate IR spectrum of the magic (MgSiO3)5 cluster. The calculated IR spectrum of the magic pyroxene cluster exhibits a number of features at wavelengths in very good agreement with the observationally derived average MAC for crystalline pyroxene, which, at the same time, cannot be explained using experimental MACs from bulk crystalline pyroxene samples. We interpret this finding as strong evidence for the existence of this particular nanodust particle around HAeBe stars. The implications of this result with respect to the properties of the associated protoplanetary disks are discussed.

[1] A. Juhász et al., "Dust evolution in protoplanetary disks around Herbig Ae/Be stars-the Spitzer view," Astrophys. J. 721, 431 (2010).

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Yes

Primary authors: Mr MACIÀ, Antoni (University of Barcelona); Prof. BROMLEY, Stefan (University of Barcelona / ICREA)

Presenter: Prof. BROMLEY, Stefan (University of Barcelona / ICREA)

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