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Nucleation, packing and beyond geometrical packing of Hard Spheres: Study using Lennard-Jones Models

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Abstract:

In first part, we study crystal nucleation by using the recently introduced Persistent Embryo Method (PEM). The method provides detailed characterization of pre-critical, critical and post-critical nuclei, as well as nucleation rates that compare favorably with those obtained using other methods (umbrella sampling, forward flux sampling or seeding). We further map our results to a hard sphere model allowing to compare with other existing predictions. Implications for experiments are also discussed.

In second part, we investigate stable structures for the mixture of hard spheres. Our results show that different types of stable structures will appear by tunneling the sizes of particles and the strength of interaction. Comparing with the strength of interaction, the type of stable structure highly depends on the sizes of particles. While the strength of interaction determines whether a certain type of structure is stable or not. Furthermore, we introduce the concept of motif to describe the relation between stable and meta-stable structures. Our results show that meta-stable structures will share the same motif with the corresponding stable structure. The concept of motif will provide a new insight into material search and material design.

**The first part of this work has been published. The second part will be submitted soon. Please refer the two papers below for more information.*

Reference:

1. S. Ren, Y. Sun, F. Zhang, A. Travasset, C.-Z. Wang and K.-M. Ho, *Soft Matter*, 2018, **14**, 9185-9193 DOI: [10.1039/C8SM01415A](https://doi.org/10.1039/C8SM01415A)
2. S. Ren, Y. Sun, F. Zhang, A. Travasset, C.-Z. Wang and K.-M. Ho, “Beyond geometrical packing of 3-D crystal structures: Study using Lennard-Jones models”, *in preparation*.