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Geometric nanoparticle model

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Nanoparticles play an increasingly significant role in chemical research primarily in the catalytic processes of chemical reactions essential for sustainable energy management. The most crucial characteristic in the application of nanoparticles is their size, from which the surface-to-volume ratio can be inferred.

In the research summarized here, we have developed a new model extending across geometrical planes for nanoparticles, primarily for interpreting thermodynamic properties. The essence of the model lies in calculating the total internal energy of nanoparticles using the spatial arrangement of monomer units with the aid of the Lenard-Jones potential (which is inversely proportional to the sixth power of the distance between two monomer units, attractive, and to the twelfth power, repulsive).

By examining the internal energy based on the spatial coordinates of monomer units within the particle and seeking the energy minimum, the most favorable geometry can be determined, primarily needed for a small number of monomer units. For particles containing a larger number of monomer units, statistical considerations are more applicable. We also investigated the case of lattice structures. It was shown that any infinite lattice displaying translational symmetry is stable concerning the Lenard-Jones potential in the sense that the local energy minimum corresponds to the lattice's geometric arrangement.

Quantum mechanical calculations were also performed. We determined the total energy and geometry of palladium nanoparticles containing an increasing number of monomer units, comparing them with the expectations of the geometric model.

Keywords: geometric kernel, nanoparticle formation, Lenard-Jones potential