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Long-range van der Waals interaction between nanoclusters[1]
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— van der Waals (vdW) interaction is an important long-range correlation that affects many properties of materials. However, this effect cannot be accurately accounted for by first-principles calculations, due to computational challenges. Recently, we have developed a model for the vdW coefficients between quasispherical clusters such as fullerenes, sodium and silicon clusters. Our study shows that the widely-used atom-pairwise interaction picture surprisingly breaks down. A quick remedy of this problem leads to a counterintuitive scaling law of the vdW coefficients for caged molecules and clusters.

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