Modeling the Emergence of Localized Surface Plasmon Resonance in Noble Metal Nanoclusters by Density-Functional Theory

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ABSTRACT

Modeling the emergence of the plasmon resonance in noble metal nanoclusters is still a challenge to tackle for theoretical chemistry. The systems are indeed too small to neglect quantum-size effects but too large to be easily assessed with quantum mechanics. In short, we present here a novel methodology based on density-functional theory (DFT) allowing for the computation and interpretation of the plasmon resonance in noble metal nanoclusters.

References

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