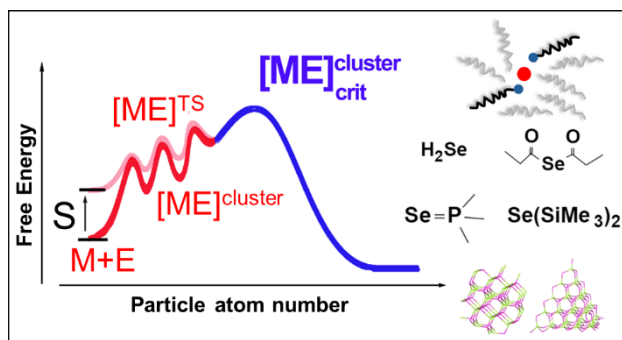


A General Nucleation Model for Semiconductor and Metallic Nanocrystals

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We introduce a nonclassical model for nanocrystal nucleation in solution which centers on the dynamic interplay of chemical bond breakage and formation coupled with the desolvation of precursor molecules, which we term the molecular chemistry (MC) model¹. Departing from classical theory, our model employs the bond count as the key variable rather than particle size, thereby redefining the role of supersaturation and its role in determining the so-called critical nucleus size. We apply the model to CdSe and Cu nanocrystals² formation in organic solvents and showcase its efficacy in predicting solvent dynamics, precursor characteristics, crystal phase, stoichiometry, “magic number” behavior, and shape control. While the electronic structure methods are used to determine the bond energy, we show that it is possible to derive reaction pathways by reducing the calculations to algebraic approximations for the nucleation energy. This singular set of bond energy parameters allows nanocrystal nucleation and growth to be conceptualized as a straightforward chemical reaction.



[1] Z. Chen, S. P. Russo, P. Mulvaney, *J. Am. Chem. Soc.* **2024**, 146, 21600–21611.

[2] Z. Chen, L. ZaZa, A. Loiudice, P. Mulvaney, R. Buonsanti, in preparation.