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Dynamic fluctuations in ultrasmall nanocrystals induce white light emission TIMOTHY J. PENNYCOOK, JAMES R. MCBRIDE, SANDRA J. ROSENTHAL, Vanderbilt University, STEPHEN J. PENNYCOOK, Oak Ridge National Laboratory, SOKRATES T. PANTELIDES, Vanderbilt University — Nanocrystals typically emit monochromatically at their size-dependent energy gaps. Recently, it was found that by pushing the size of a nanocrystal to its lower limits, absorption occurs at increasingly larger energies, but the expected blue to ultraviolet emission does not occur. Instead, ultrasmall nanocrystals begin to emit a broader spectrum. For instance, ultrasmall CdSe nanocrystals emit white light [1]. We have investigated small to ultrasmall CdSe nanocrystals using a combination of state-of-the-art scanning transmission electron microscopy and finite-temperature quantum molecular dynamics simulations. Our findings indicate that following excitation, partial thermalization sets the ultrasmall nanocrystals into a fluxional state, with a continuously varying energy gap, which results in white light emission when averaged over time. Furthermore, although the larger monochromatic emitting nanocrystals we have observed possess stable crystal cores, their surfaces are fluxional. Dynamic fluxionality should be taken into consideration when optimizing nanocrystals for applications. This work is supported by DOE grant DE-FG02-09ER46554 and Basic Energy Sciences Materials Sciences and Engineering Division.

[1] Bowers II, M.J. et al. J. Am. Chem. Soc 127, 15378 (2005).

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