Mesoscale Priority Research Direction

Fluctuation de/stabilization of mesoscale structures

Opportunity

Thermal fluctuation effects are well recognized in van der Waals (vdW) interactions but not in other types of long-range interactions. How does thermal noise fluctuation work with conformational, electrostatic, and solvent structure (polar) interactions to stabilize/destabilize soft nanoscale structures? What compound effects of thermal fluctuations span all scales?

Mesoscale Challenge

The meso challenges are:

i) to understand the coupling between thermal effects on various levels of long range interaction description

ii) to control thermal effects in one type of interaction (e.g., electrostatic) by modifying the properties of another one (e.g., optical spectra in vdW)

iii) to distinguish, discern, characterize fluctuation effects on all spatial scales.

iv) to understand the time evolution of the system's fluctuations and stability

Approach

Calculate the thermal noise effects on electrostatic interactions, solvent structure (polar) interactions and van del Waals interactions that dominate stability properties. Fluctuations have different levels of action: conformational fluctuations modify optical spectra that modify the vdW interaction that modifies the structural interaction. Working in a statistical mechanics and thermodynamic free energy framework, we evaluate the net total effect of fluctuations at all levels of description.

Impact

The largest lengthscale effects of fluctuations are those that govern the stability of these technologically important structures. Working with material structures on the nano-, meso- and macro- lengthscales, one needs to know the total effect of thermal fluctuations, seeing all lengthscales available to the system. Partial effects on one lengthscale can be modified/reversed when longer lengthscales are incorporated.

References: Roger H. French, V. Adrian Parsegian, Rudolf Podgornik et al. Long Range Interactions in Nanoscale Science, Reviews of Modern Physics, 82, 1887 (2010).

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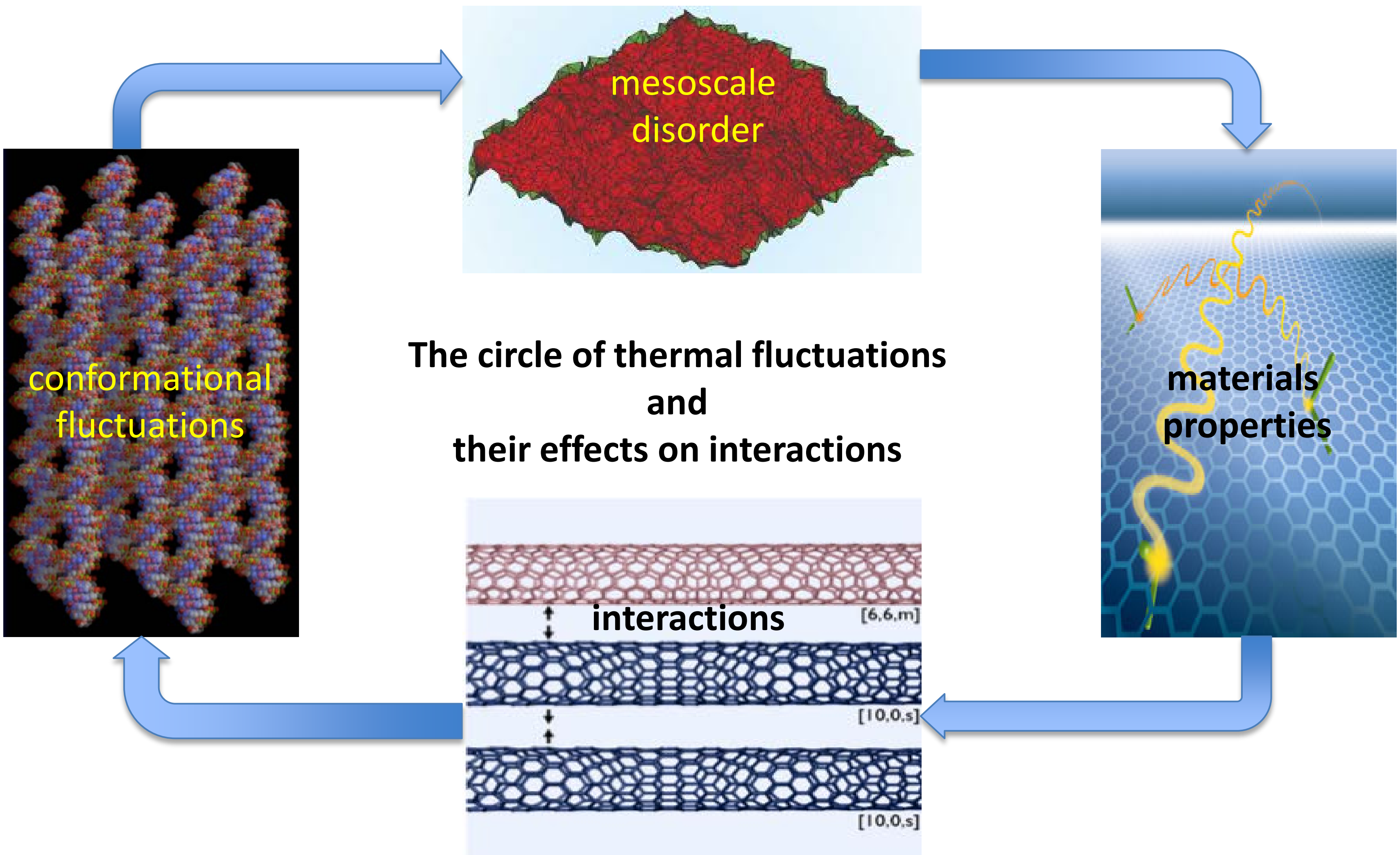

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