Seminar/Talk

Many-particle limits in molecular solvation

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Host: Jan Maas

We present a variational model of the solvation of biological macromolecules, e.g. proteins, in cells. We identify different energy scaling laws and different phases depending on the number of molecules as the ratio between cell size and molecule size tends to infinity, and observe a local-nonlocal transition of the limit energy as molecule number passes a critical threshold: the solvent is able to suppress long-range Coulomb interactions only for a certain charge density. This screening effect becomes much stronger in the presence of the common-ion effect. This is reflected in multiple Gamma-convergence theorems. Joint work with Janusz Ginster (Carnegie Mellon University).

Thursday, January 25, 2018 04:00pm - 06:00pm
Big Seminar room Ground floor / Office Bldg West (I21.EG.101)

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