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Polarizability, susceptibility, and dielectric constant of nano-scale molecular films: a microscopic view AMIR NATAN, NATALIA KURITZ, LEEOR KRONIK, Weizmann Institute of Science, Israel — We explore theoretically the size-dependence of the polarizability, susceptibility, and dielectric constant of nano-scale molecular layers. This is achieved by comparing first principles calculations based on density functional theory to phenomenological modeling based on polarizable dipolar arrays, for a model system of organized monolayers comprised of oligophenyl chains. We show that molecular packing density is the single most important factor controlling the bulk limit of all three quantities as well as the rate at which they are approached. Finally, we show that the polarization does not reach its "bulk" limit, as determined from the Clausius-Mossotti (CM) model, but the susceptibility and dielectric constant do converge to the correct bulk limit. However, whereas the CM model describes the dielectric constant well at low lateral densities, finite size effects of the monomer units cause it to be increasingly inaccurate at high lateral densities.

Amir Natan
Weizmann Institute of Science, Israel

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