

Density functional theory for nanoparticles at liquid-liquid interfaces

S. Sokółowski^a and O. Pizio^b

^a*Department for the Modelling of Physico-Chemical Processes, Maria Curie-Skłodowska University, Lublin 20-031, Poland,*

E-mail: stefan.sokolowski@gmail.com

^b*Instituto de Química, Universidad Nacional Autónoma de México, Circuito Exterior, 04510, Cd. de México, México*

E-mail: pizio@unam.mx

We propose an extension of density functional approach to study the structure and thermodynamic properties of the system comprising a certain amount of nanoparticles at the interface between two partially miscible liquids. Model calculations have been carried out for a binary symmetric mixture of hard-sphere Yukawa fluids and for spherical, as well as for dimer nanoparticles. Despite simplicity, the model captures principal features of this type of systems. The results indicate that nanoparticles form layers and the number of the layers depends on the amount of nanoparticles and on their diameters. For the systems studied the formation of the layers evidences a strong localization of the nanoparticles at the interface. In the case of dimers we have also used the site superposition approximation to evaluate the angular-dependent density profiles