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**Adhesion of Nanoparticles**[1] JAN-MICHAEL CARRILLO, University of Connecticut, ELIE RAPHAEL, ESPCI, ANDREY DOBRYNIN, University of Connecticut — We have developed a new model of nanoparticle adhesion which explicitly takes into account the change in the nanoparticle surface energy. Using combination of the molecular dynamics simulations and theoretical calculations we have showed that the deformation of the adsorbed nanoparticles is a function of the dimensionless parameter $\beta \propto \gamma\,(GR)^{-2/3}\,W^{-1/3}$, where $G$ is the particle shear modulus, $R$ is the initial particle radius, $\gamma$ is the polymer interfacial energy, and $W$ is the particle work of adhesion. In the case of small values of the parameter $\beta$ <0.1, which is usually the case for strongly cross-linked large nanoparticles, the particle deformation can be described in the framework of the classical Johnson, Kendall, and Roberts (JKR) theory. However, we observed a significant deviation from the classical JKR theory in the case of the weakly cross-linked nanoparticles that experience large shape deformations upon particle adhesion. In this case the interfacial energy of the nanoparticle plays an important role controlling nanoparticle deformation. Our model of the nanoparticle adhesion is in a very good agreement with the simulation results and provides a new universal scaling relationship for nanoparticle deformation as a function of the system parameters.

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