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Silvina Tomassone received her BS in Physics from The University of Buenos Aires and a MS and Ph. D degrees in Physics from Northeastern University (Boston). During her Ph.D. she worked on Friction at the atomic level and, later, as a postdoctoral researcher at City College of New York, she worked on Surfactant Dynamics. In 2001 she joined the faculty of Rutgers University. She is a tenured Associate Professor in the Chemical Engineering Department and a member of the graduate Faculty in the Departments of Biomedical and Mechanical Engineering. Professor Tomassone has over twelve years of experience in modeling of particulate and molecular systems. She continues to work in modeling and since joining Rutgers in 2001, she has been working in experimental nanoparticle synthesis and production. She is the author of over 60 publications in prestigious journals and more than 120 presentations at scientific conferences and invited talks. She is also the co-director of the awarded IGERT on Nanopharmaceutical Engineering.

“Multiscale Molecular Simulations on the Dispersion and Rheology of Silica Nanoparticles in a Polyethylene Melt”

In this work, a novel approach for determining the shear viscosity and dispersion/agglomeration properties of polymer nano-composites has been developed. This work is combines a novel multiscale modeling approach, with both atomistic and coarse grained simulations along with thermodynamics concepts to efficiently represent and study these systems. Silica nanoparticles in a polyethylene melt were explored as a case study, where the solid-fluid interaction parameters were determined by iterating the value of the surface tension between the silica and polyethylene at a spherical interface using thermodynamic concepts.

The viscosity of polymer nanocomposite was also calculated and it was observed that it increases up to 2 orders of magnitude when nanoparticles are included, with respect to the viscosity of a composite made out of micron sized particles. In fact, when nanoparticles are included in the polymer melt, there is a clear breakup of the Einstein-Batchelor relationship, which is valid for dilute suspensions (and valid for regular micron sized composites). In addition to the large enhancement in viscosity, it is observed that nanoparticles form chain bridging with the polymer chains, therefore contributing to the eventual formation of an amorphous solid, typical of these materials. Over the range of shear rates studied, the shear viscosity is strongly dependent on the shear rate. These trends are quantified by a power-law, which has been also verified experimentally. The viscosity of the composite is also sensitive to the size of the filler particles. Decreasing the size of spherical filler particles while keeping the filler volume fraction constant leads to an increase of the viscosity. In addition, the viscosity of the melt was studied as a function of the polymer chain length, nanoparticle size, and fill fraction of the particles. It was found that the shear viscosity consistently increased with an increased concentration of particles. Furthermore, it was found that a thermodynamically stable dispersion of nanoparticles was established when the radius of gyration of the linear polymer was greater than the radius of the dispersed nanoparticles. These findings show good agreement with experimental studies reported in the literature.