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Path-Integration Computation of the Transport Properties of Nanoparticles JACK DOUGLAS, NIST — There is need for effective computational methods for calculating the transport properties of polymers and complex-shaped particle aggregates arising in materials science and biology as a foundation for rational material design and the design of well-defined measurements assessing the environmental impact of nanoparticles. We focus on the problem of calculating basic solution transport properties (translational diffusion coefficient, intrinsic viscosity) of isolated particles having essentially any geometry using a novel computational method involving path integration developed by Mansfield and Douglas. The basic concepts behind the method are described and the method is validated in cases where exact analytic, or at least highly accurate numerical estimates, are known for comparison. After defining and validating our method, some applications of the program are given to some non-trivial problems illustrating the use of the program for charactering such as nanoparticles with grafted DNA brush layers, DNA orgami, carbon nanotubes, etc. The path-integration method is evidently a powerful tool for computing basic transport properties of complex-shaped objects and should find wide application in polymer science, nanotechnological applications and biology.

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