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Optical Properties of Molecular Dots TIMOTHY RUSSIN<sup>1</sup>, GU-GANG CHEN, JAMES ADAIR<sup>2</sup>, PETER EKLUND<sup>3</sup>, The Pennsylvania State University — A "Molecular Dot" (or "M-dot") refers to a mixed organic/inorganic phase of nanomatter where a small number of organic molecules are encapsulated in an inorganic nanoparticle. Particular interest has been initiated in these systems when the molecules exhibit photoluminescence (PL) and the nanoparticle provides a transparent medium allowing easy entrance and exit of photons. They show promise for medical applications. In preliminary experimental studies, the encapsulation has been found to enhance the PL and suppress the photo-degradation of organic dye molecules such as Rhodamine B encapsulated in  $SiO_2$  or CaPO<sub>4</sub>. In this paper, we present the results of an optical model to predict the optical properties of M-dots. Using the discrete dipole approximation, we take into account the effects of Mie scattering and the effective dielectric function of the dye molecules encapsulated in an inorganic host of known refractive index. The results of the modeling will be compared to recent experimental results on M-dots in dilute solution, i.e., optical absorption and dispersion in the NIR-Vis-UV regions.

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