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Computational Study for the Prediction of Optical Properties of Polymer

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Computational study has been conducted to predict optical properties of polymers. We developed a practical strategy to predict birefringence of crystalline and non-crystalline polymer by using quantum mechanical calculation and statistical approach. The basic idea is conventional one, which estimates the birefringence from polarizability by Lorentz-Lorenz equation. However, we studied a various calculation conditions such as the Hamiltonian of quantum mechanical calculation and the criteria of the selection of conformation. As the results of the study, we obtained the strategy that gives acceptable accuracy of birefringence of polymers to help the design optical materials with reasonable computational time. We also studied optoelastic coefficient of amorphous polymer such as polystyrene (PS) by using force field calculation and bond polarizability method. The results reproduced the experimental results qualitatively. Furthermore, the conformational change at the small deformation is studied in the details.