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Accelerated Discovery of High-Refractive-Index Polymers Using First-Principles Modeling, Virtual High-Throughput Screening, and Data Mining MOHAMMAD ATIF FAIZ AFZAL, CHONG CHENG, JOHANNES HACHMANN, State University of New York, University at Buffalo — Organic materials with refractive index (RI) values higher than 1.7 have attracted considerable interest in recent years due to the tremendous potential for their application in optical, optometric, and optoelectronic devices, and thus for shaping technological innovation in numerous related areas. Our work is concerned with creating predictive models for the optical properties of organic polymers, which will guide our experimentalist partners and allow them to target the most promising candidates. The RI model is developed based on a synergistic combination of first-principles electronic structure theory and machine learning techniques. The RI values predicted for common polymers using this model are in very good agreement with the experimental values. We also benchmark different DFT approximations along with various basis sets for their predictive performance in this model. We demonstrate that this combination of first-principles and data modeling is both successful and highly economical in determining the RI values of a wide range of organic polymers. To accelerate the development process, we cast this modeling approach into the high-throughput screening, materials informatics, and rational design framework that is developed in the group. This framework is a powerful tool and has shown to be highly promising for rapidly identifying polymer candidates with exceptional RI values as well as discovering design rules for advanced materials.

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