Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Accurate prediction of the refractive index of polymers using first principles and data modeling MOHAMMAD ATIF FAIZ AFZAL, CHONG CHENG, JOHANNES HACHMANN, State Univ of NY - Buffalo — Organic polymers with a high refractive index (RI) have recently attracted considerable interest due to their potential application in optical and optoelectronic devices. The ability to tailor the molecular structure of polymers is the key to increasing the accessible RI values. Our work concerns the creation of predictive *in silico* models for the optical properties of organic polymers, the screening of large-scale candidate libraries, and the mining of the resulting data to extract the underlying design principles that govern their performance. This work was set up to guide our experimentalist partners and allow them to target the most promising candidates. Our model is based on the Lorentz-Lorenz equation and thus includes the polarizability and number density values for each candidate. For the former, we performed a detailed benchmark study of different density functionals, basis sets, and the extrapolation scheme towards the polymer limit. For the number density we devised an exceedingly efficient machine learning approach to correlate the polymer structure and the packing fraction in the bulk material. We validated the proposed RI model against the experimentally known RI values of 112 polymers. We could show that the proposed combination of physical and data modeling is both successful and highly economical to characterize a wide range of organic polymers, which is a prerequisite for virtual high-throughput screening.

Mohammad Atif Faiz Afzal
State Univ of NY - Buffalo

Date submitted: 23 Nov 2015 Electronic form version 1.4