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A Multi-Objective Optimization Technique to Model the Pareto Front of Organic Dielectric Polymers[1] J. E. GUBERNATIS, Theoretical Division, Los Alamos National Laboratory, A. MANNODI-KANAKKITHODI, R. RAMPRASAD, Department of Materials Science and Engineering, University of Connecticut, G. PILANIA, Materials Science and Engineering Division, Los Alamos National Laboratory, T. LOOKMAN, Theoretical Division, Los Alamos National Laboratory — Multi-objective optimization is an area of decision making that is concerned with mathematical optimization problems involving more than one objective simultaneously. Here we describe two new Monte Carlo methods for this type of optimization in the context of their application to the problem of designing polymers with more desirable dielectric and optical properties. We present results of applying these Monte Carlo methods to a two-objective problem (maximizing the total static band dielectric constant and energy gap) and a three objective problem (maximizing the ionic and electronic contributions to the static band dielectric constant and energy gap) of a 6-block organic polymer. Our objective functions were constructed from high throughput DFT calculations of 4-block polymers, following the method of Sharma et al., Nature Communications 5, 4845 (2014) and Mannodi-Kanakkithodi et al., Scientific Reports, submitted. Our high throughput and Monte Carlo methods of analysis extend to general N-block organic polymers.

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J. E. Gubernatis
Theoretical Division, Los Alamos National Laboratory

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