Prediction of novel single-layer materials for device applications
BENJAMIN C. REVARD, WILLIAM W. TIPTON, RICHARD G. HENNIG, Cornell University — Single-layer materials represent a new materials class with potentially transformative properties for applications in nanoelectronics and solar energy harvesting. With the goal to discover novel 2D materials with unusual compositions and structures, we have developed a grand-canonical evolutionary algorithm for two-dimensional materials. Here we present the details of the algorithm and our initial results. Using both empirical and first principles total energy methods in the evolutionary algorithm, we show that the method can successfully identify known structures of 2D materials such as graphene and graphane. We currently apply the approach to a number of other promising candidate systems and will report the findings.

Richard G. Hennig
Cornell University