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First principles characterization of novel single-layer materials predicted with an evolutionary algorithm[1] BENJAMIN REVARD, WILL TIPTON, Department of Materials Science and Engineering, Cornell University, RICHARD HENNIG, Department of Materials Science and Engineering, University of Florida — 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 unexpected compositions and structures, we have developed a grand-canonical evolutionary algorithm for two-dimensional materials. Here we present the results of applying the algorithm, coupled with first principles total energy methods, to several technologically relevant binary 2D systems, including C-Si, Sn-S and PbO. We currently use computational techniques to characterize the vibrational and electronic properties of the low energy 2D materials predicted by the algorithm and will report the findings.

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