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ADMIRAL framework- Advanced Data-Mining for Improved Research And Learning

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We have developed a software which incorporates genetic algorithms, neural networks and methods of data-mining for research and development of materials at atomic scale. Application of the software on research of energetically most favorable doping configurations of magnesium hexaboride will be presented. We demonstrate an efficient search for global minimum in the configuration space utilizing crossover and mutation genetic operators that are finely optimized for the particular system.

Symposium D4.I: Combinatorial and High-Throughput Methods