



Combi

Starting from a parent structure this module generates a combinatorial set of different structures, enters them into a MedeA spreadsheet and then allows the calculation of properties such as a binding energy or magnetic moments. The Combi module is a very convenient tool to organize large sets of similar calculations for exhaustive explorations ("grid searches") in a design space.

Results from Combi

- ▶ Spreadsheet with system name, composition, and computed parameters
- ▶ Simple export of MedeA spreadsheet to Excel

Computational characteristics

- ▶ Choice of computational program (e.g. VASP 4.6 or VASP 5.2)
- ▶ Automatic and consistent setting of computational parameters across the entire set of systems

Required MedeA modules

- ▶ [Core MedeA environment](#)
- ▶ [MedeA VASP 4.6 or 5.2](#)
- ▶ [Job Server and Task Servers](#)

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