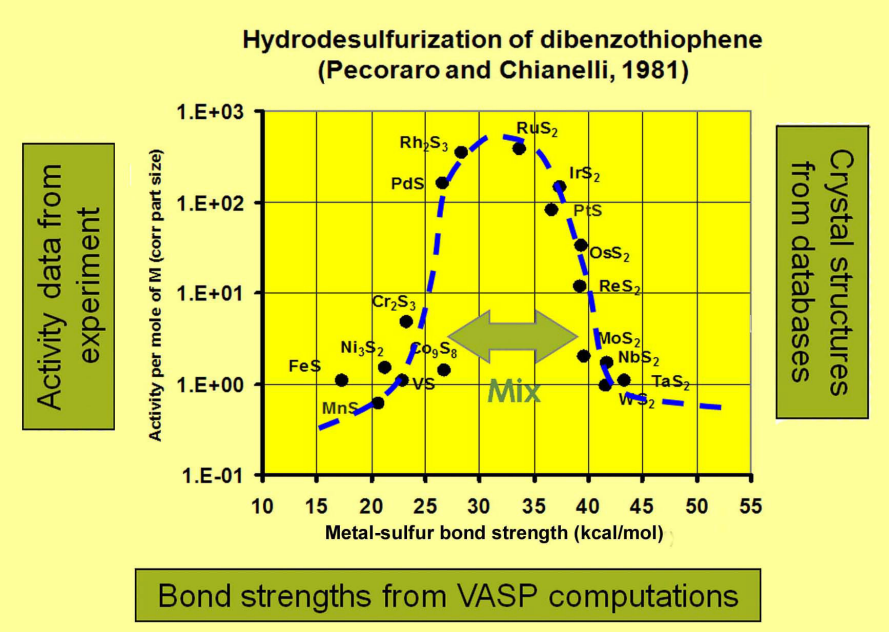
PrediBond™

This module is the result of a collaborative effort between the French Petroleum Institute and Materials Design. It uses a patented approach to screen and rank a range of materials according to their binding strength with specific target atoms. This approach has been used, for example, in the screening of catalytic materials for the hydro-desulfurization of fuel feedstock. The approach is more generally applicable to any question where bonding strength of a material to specific elements plays a decisive role. This includes, for example, the immobilization of radioactive elements in an oxide matrix.



Catalytic activity vs. bond strength computed with PrediBond™ revealing a volcano-curve correlation. Combinations such as MoS_2 and Ni_3S_2 lead to the desired optimal activity.

Results from PrediBond™

- Spreadsheet with system name, composition, and computed parameters for a list of candidate materials
- Ranking of candidate materials according to bond strength
- Simple export of MedeA spreadsheet to Excel

Computational characteristics

- Choice of computational program (e.g. VASP 4.6 or VASP 5.2)
- Choice of target atoms
- Combinatorial creation of possibility candidates
- 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

More on our website:

www.materialsdesign.com

- Screening of desulfurization catalysts

Relevant Publications

- H Toulhoat, US Patent 6799089, Sep. 28, 2004
- P Raybaud, *Applied Catalysis A: General* vol. 322 p. 76-91, 2007
- H Toulhoat, *Journal of Catalysis* vol. 216 (1-2) p. 63-72, 2003

Note

- License of PrediBondTM entitles the user to use the patented algorithm : (US Patent 6799089)