Ab initio and thermodynamic investigations of complexion-forming systems

Plan of work:
Create database of physical properties from first-principles
Fit parameterized potentials
Deliver potentials for molecular dynamics simulations
Utilize potentials for complexion phase diagram prediction

Year 1:
Develop two- and three-body potential for alumina
Begin study of complexion thermodynamics and phase diagrams
Years 2&3:
Develop EAM-type potentials for metallic systems such as Ni-Bi
Explore classical liquid DFT-based approach to phase field models
Continue study of complexion phase diagrams

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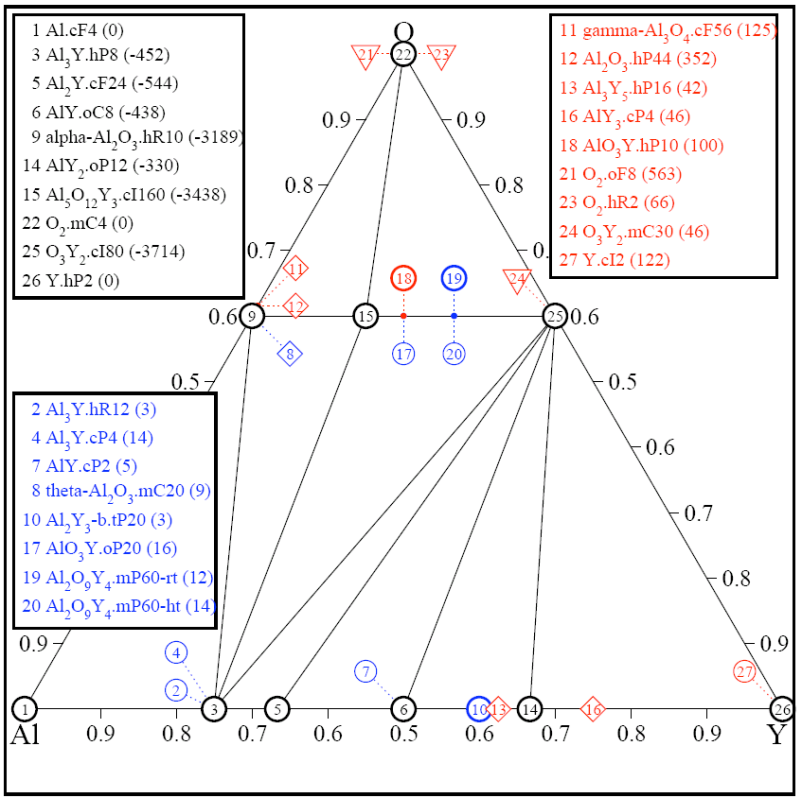
Enthalpies of formation
example: Y-doped alumina



Elasticity
example: α-Al_2O_3

Elastic constant (GPa)	Experiment (T=25 C)	Calculation (T=0 K)
C11	498	562
C12	163	192
C13	117	159
C14	-23	19.7
C33	502	549
C44	147	176
C66	167	185