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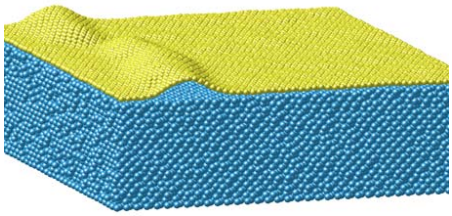
Research interests: computational materials science, thermodynamics & kinetics, phase transformations, prediction of materials properties

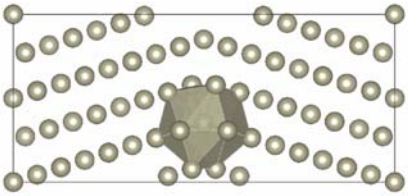
Virtual Materials

Recent Research activities:
Molecular Dynamics simulation of wrinkles in graphene grown on copper (with TPC Klaver).



Wrinkled graphene (yellow) on Cu (blue) substrate

Twinning in hcp metals



Model of "unusual" {1121} twin with distorted icosahedral coordination polyhedron.
The exceptional ductility of Re-based alloys was explained. Currently work under way to apply this understanding to design of ductile hcp high entropy alloys (with M de Jong).

Development of a software module for efficiently predicting elastic tensor of arbitrary compounds (with M. de Jong).

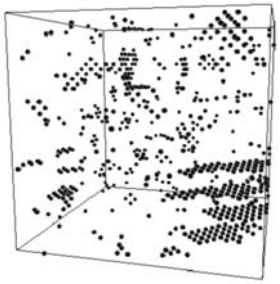
$$\begin{Bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \sigma_4\\ \sigma_5\\ \sigma_6\end{Bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ & & C_{33} & C_{34} & C_{35} & C_{36} \\ & & & C_{44} & C_{45} & C_{46} \\ & Sym. & & & C_{55} & C_{56} \\ & & & & & C_{66} \end{bmatrix} \begin{Bmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \varepsilon_4\\ \varepsilon_5\\ \varepsilon_6\end{Bmatrix}$$

Details at: http://www.materialsproject.org/

Tuning magnetic properties of high entropy alloys. Ab initio calculations of the disordered local moment model lead to mapping the Curie temperature – composition relation in multicomponent alloys (with F Kormann).

A theory for the vacancy formation energy in concentrated alloys was formulated and applied to Cu-Ni alloys (with X Zhang).

Ab initio prediction of the kinetics of the earliest stages of precipitation in Al-Cu alloys with a realistic time scale (with X Zhang).



Kinetic Monte Carlo model simulation of GP-I to GP-II transition in an Al 2 a/o Cu alloy.

Key publications (2015):
M. de Jong et al., Nature Sci. Data 2, 1-13.
M. de Jong et al., Phys. Rev. Lett. 115, 065501.
F. Kormann et al., Appl. Phys. Lett. 107, 142404.
http://tinyurl.com/hb8gwhw

Other Achievements (2015):
Invited talks at TMS (Orlando), ICAMS (Bochum), ESTADSM (Moscow), KTH (Stockholm)
CVM workshop organized & hosted in Delft (July)