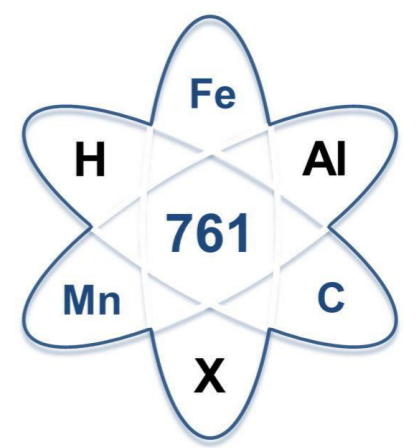


# A2 *Ab initio* Thermodynamics and Kinetics

Calculation of free energies, stacking fault and grain boundary energies at evaluated temperatures

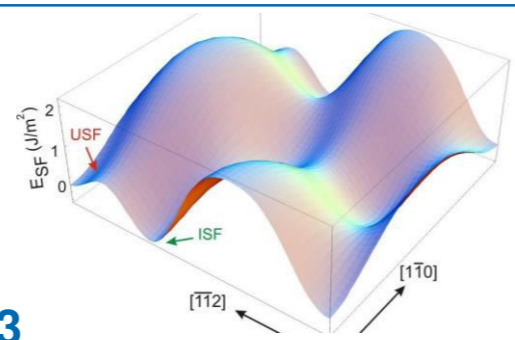


Ivan Bleskov, Fritz Körmann, Tilmann Hickel  
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## Results of the 2nd phase

### Motivation

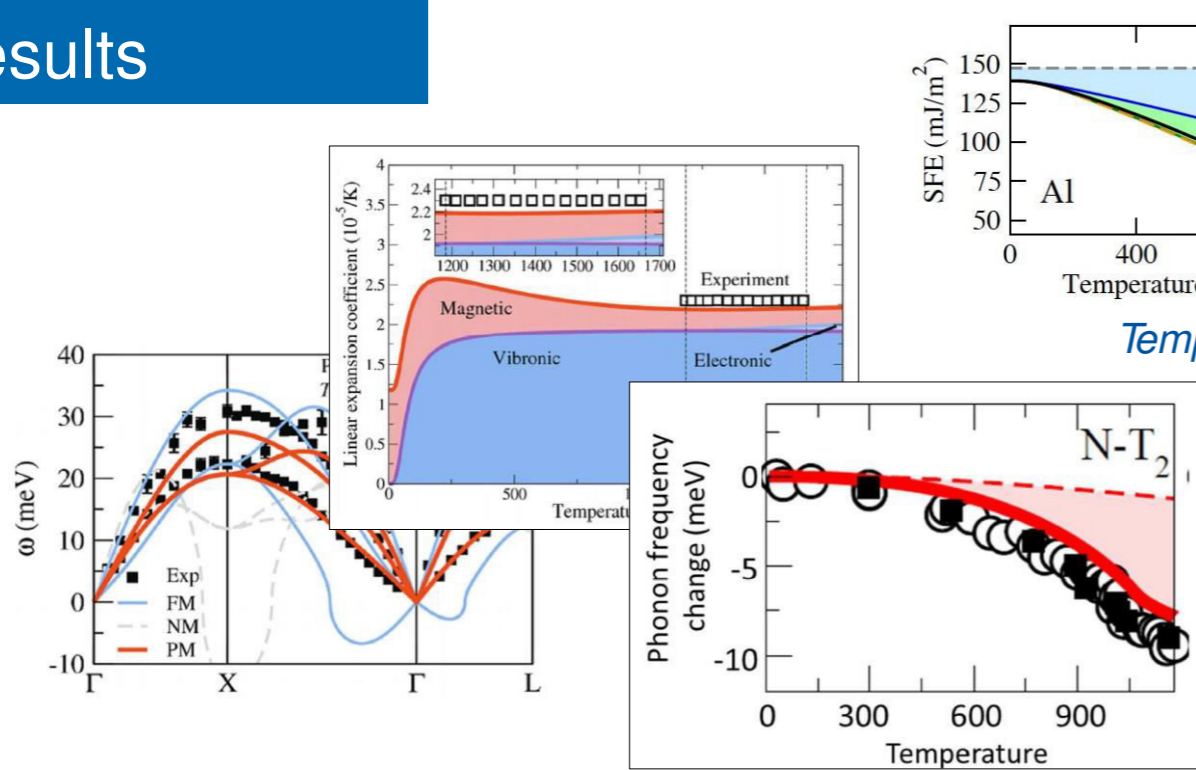
- ab initio* Thermodynamics
  - Fundamental understanding of materials properties
  - Thermodynamic modelling → **A3**
- Stacking fault (SF) energies calculations
  - Deformation mechanisms / exp. phenomena
  - Chemical trends, e.g. carbon → **A5, A7, B1**
- Grain boundaries
  - Twin boundaries → understanding from HR-TEM → **C1**
  - Obstacles for dislocations movement → **A7, A10**
- Kinetics, e.g. nanodiffusion near the SF
  - Understanding of TEM experiments → **C10**



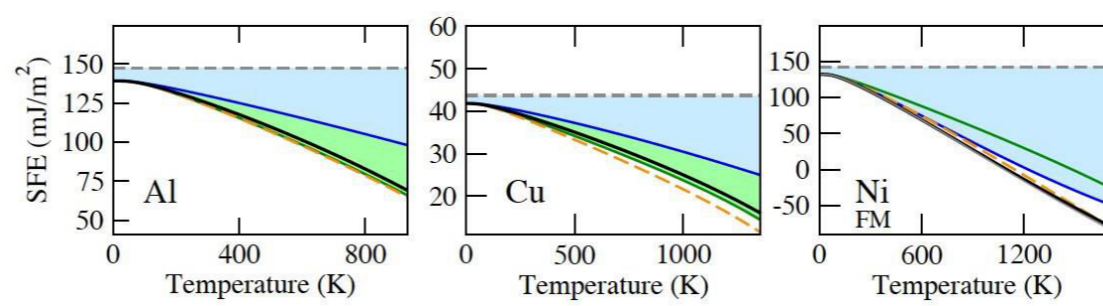
### Methods

- Density functional theory (DFT)
  - Exact MT-orbitals method
  - Projected augmented waves (VASP code)
- Chemical / magnetic disorder
  - Special quasirandom structures (SQS)
  - Coherent potential approximation (CPA)
  - Disordered local moments (DLM) approximation
  - Spin space averaging (SSA) method
- (Generalized) stacking fault / twin energy
  - Explicit supercell approach
  - Axial next nearest neighbour Ising (ANNNI) model
- Kinetics / diffusion barriers
  - Nudged elastic band method

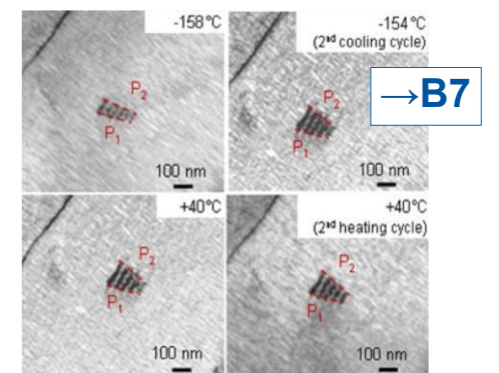
### Results



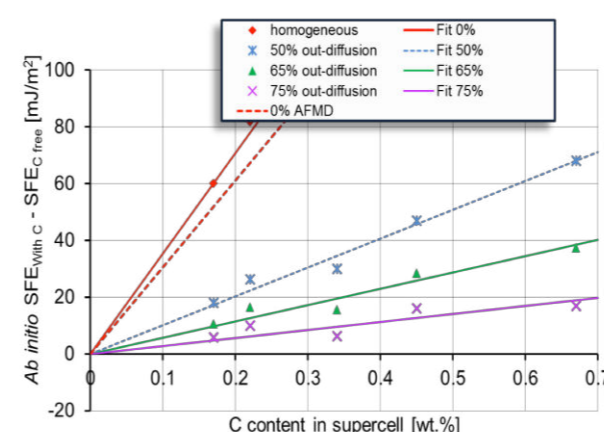
Influence of local magnetism on thermodynamic properties



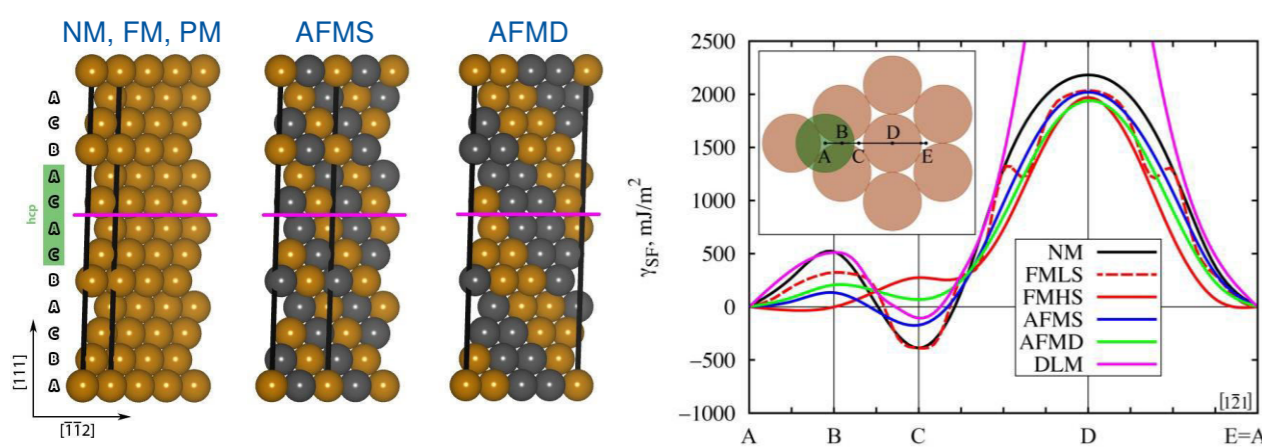
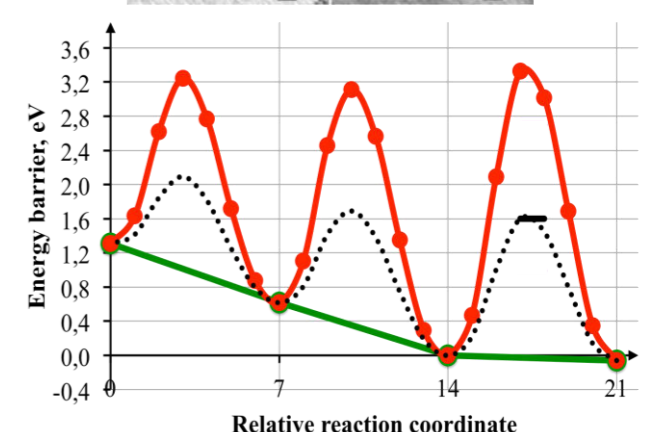
Temperature dependence of the SFE



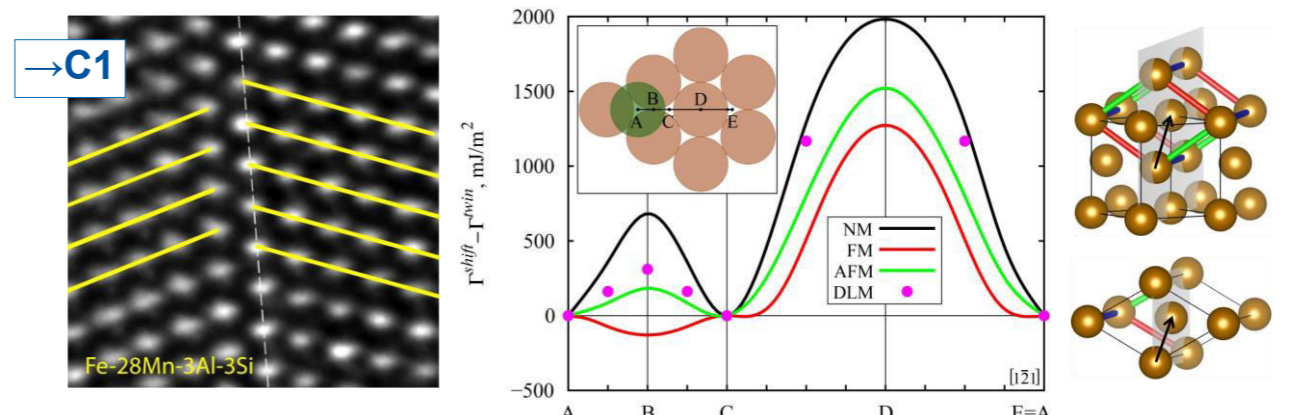
→ **B7**



Influence of nano-diffusion on the chemical trends of the SFE



Influence of local magnetism on the GSFE surface in Fe



Shift of atomic layers on the twin boundary: local magnetism

### Impact

- Impact for the SFB:
  - Important contribution to the multi-scale simulations of deformation mechanisms
  - D.R.Steinmetz, T.Jäpel, B.Wietbrock, P.Eisenlohr, I.Gutierrez-Urrutia, A.Saeed-Akbari, T.Hickel, F.Roters, D.Raabe: Acta Mater 61 (2013) 494
  - Understanding of experimental results such as the behaviour of twin boundaries
- Impact for the (worldwide) scientific Community:
  - New methodology (SSA) for the atomic forces calculation at evaluated magnetic temperatures
  - F. Körmann, B. Grabowski, B. Dutta, T. Hickel, L. Mauger, B. Fultz, and J. Neugebauer: PRL 113 (2014) 165503
  - The influence of local effects (chemical composition, pressure, magnetism) on the SFE
  - T. Hickel, S. Sandlöbes, R.K.W. Marceau, A. Dick, I. Bleskov, J. Neugebauer, D. Raabe: Acta Mater 75 (2014) 147-155

