# Thermodynamics and Kinetics-driven Dual States in FeMn(PSi) Alloys

**Guijiang Li,[1] Levente Vitos[1,2,3]**
[1]*Applied Materials Physics, Department of Materials Science and Engineering, KTH Royal Institute of Technology, Stockholm, Sweden*
[2]*Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Uppsala, Sweden*
[3]*Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Budapest, Hungary*
*levente@kth.se*

$Fe_2P$-type alloys have been an interesting research topic because of the potential application as magneto-caloric materials and also because of the rich physical properties for fundamental research. We have investigated the magnetic exchange interactions, microscopic theory of magnetism, magneto-elastic effect, the magneto-structural coupling in $Fe_2P$-type alloys as well as the phase stability of FeMnPSi alloys.

Here we report on thermodynamic-state and kinetic-process dependent dual magnetic states in FeMn(PSi) alloys. Our investigations are based in density functional theory formualted within the exact muffin-tin orbitals method in combination with the coherent potential approximation. We identify both ferromagnetic and antiferromagnetic states in $FeMnP_{0.75}Si_{0.25}$ [1] and confirm the co-existence of dual ferromagnetic orders in $FeMnP_{0.55}Si_{0.45}$ [2]. We discuss that the thermodynamic state in the high temperature paramagnetic phase and the kinetic diffusion process upon cooling co-determine the magnetic order at low temperature. The results suggest that careful control of the kinetic diffusion process in FeMnPSi alloys serves as a another tuning parameter when searching for new magnetocaloric candidate materials.

**Key Words:** magnetocaloric, FeMnPSi, density functional, alloy theory

**References**

[1] Kinetic arrest induced antiferromagnetic order in hexagonal $FeMnP_{0.75}Si_{0.25}$ alloy. G. Li, W. Li, S. Schnecker, X. Li, E. K. Delczeg-Czirjak, Y. O. Kvashnin, O. Eriksson, B. Johansson and L. Vitos, Applied Physics Letters **105**, 262405 (2014);
[2] Thermodynamic-state and kinetic-process dependent dual ferromagnetic states in high-Si FeMn(PSi) alloys. G. Li, E. K. Delczeg-Czirjak, O. Eriksson, B. Johansson and L. Vitos, submitted.