



Comprendre le monde,
construire l'avenir®

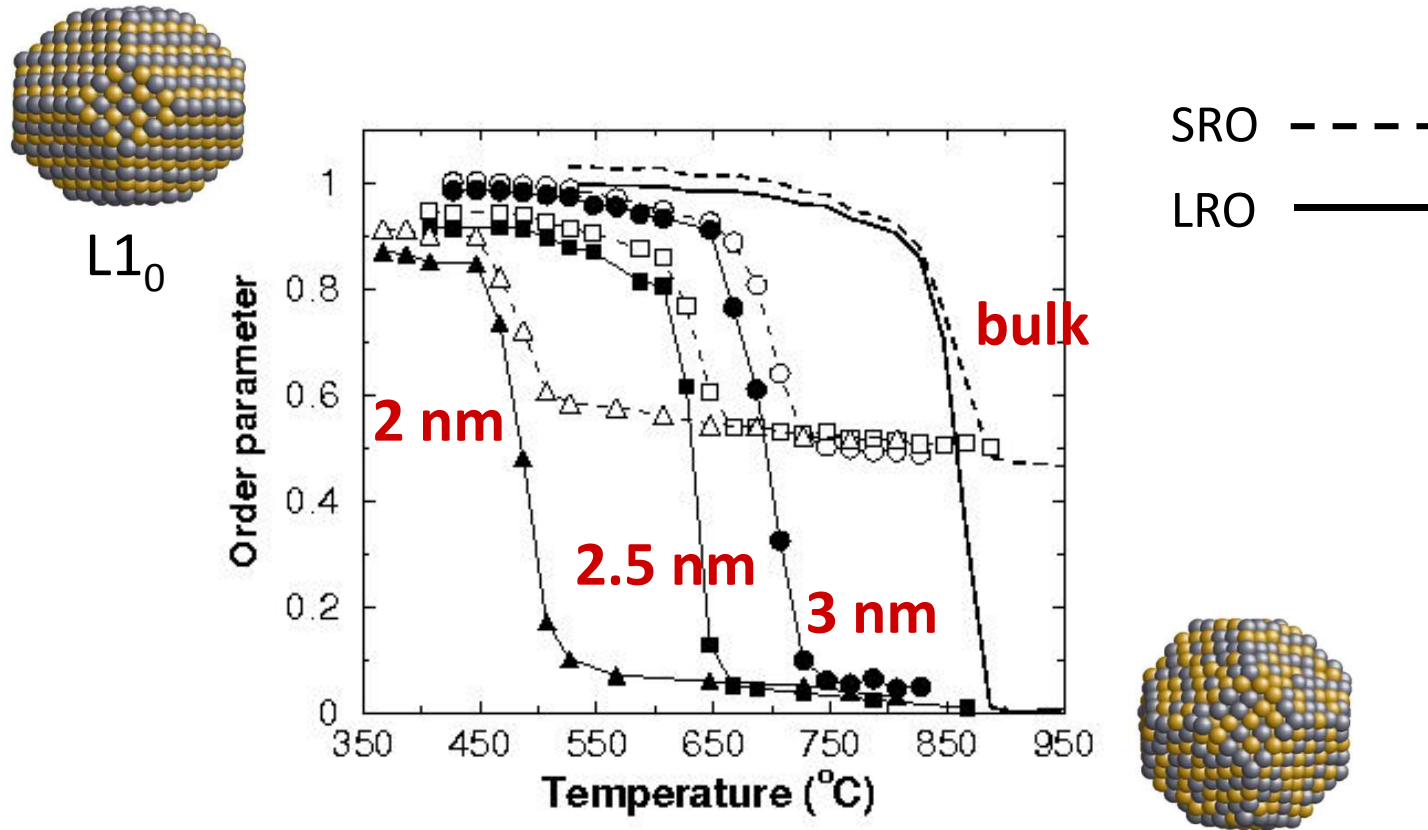
Nanowires, nanotubes, nanoalloys : a phase diagram story

F. Berthier,
A. Ziani, E. Maras,
I. Braems, J. Creuze, B. Legrand



Size and shape effects on the order-disorder phase transition in CoPt nanoparticles

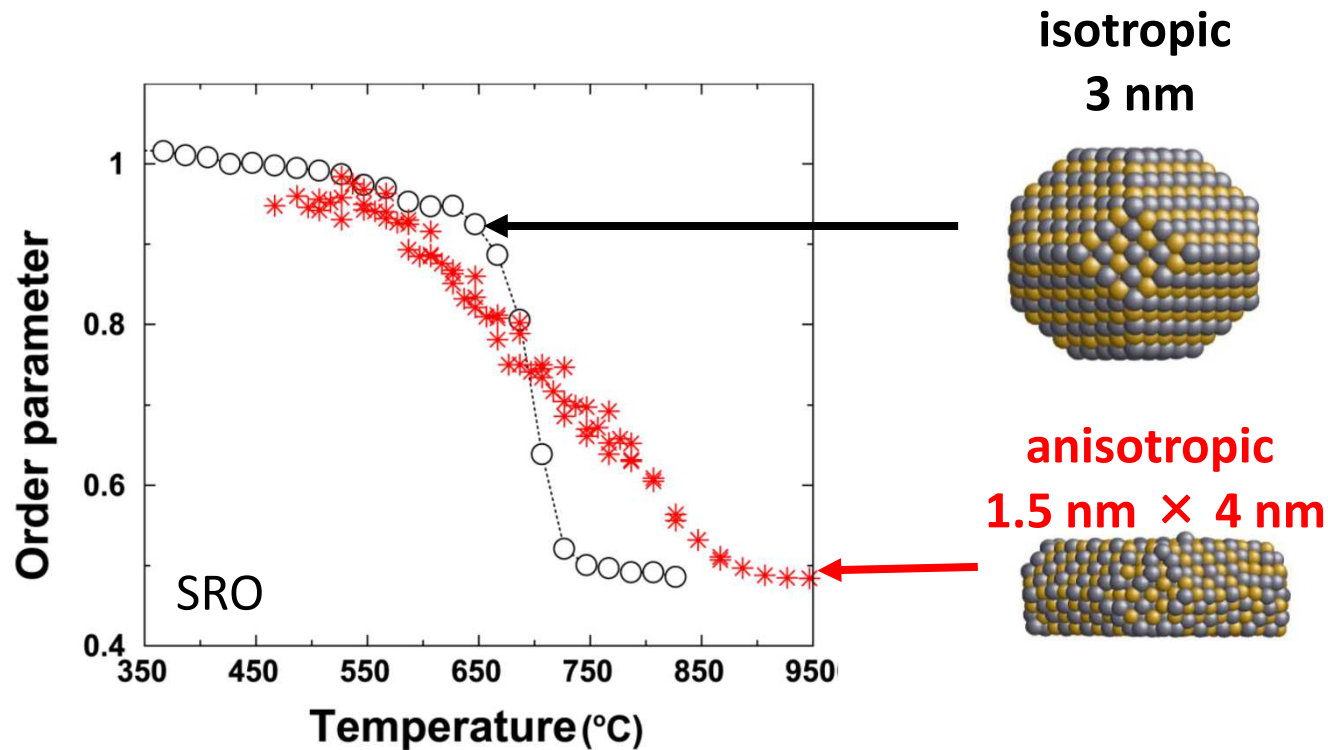
D. Alloyeau and Co., Nature Materials, 8 (2009) 940



T_c is shifted towards higher temperature with increasing cluster size

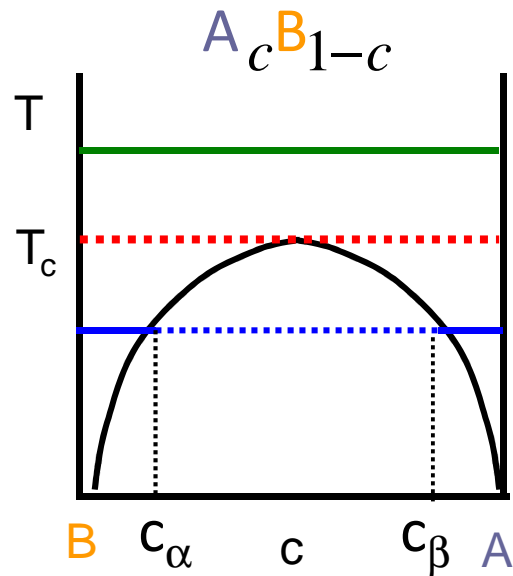
Size and shape effects on the order-disorder phase transition in CoPt nanoparticles

D. Alloyeau and Co., Nature Materials, 8 (2009) 940



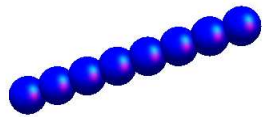
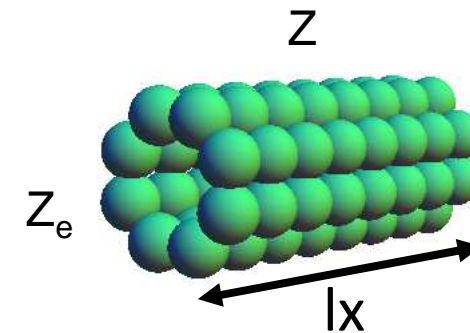
the aspect ratio affects the transition temperature of clusters

Energetic and geometric characteristics



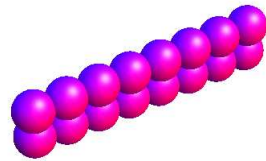
Monte Carlo simulations

$$\left\{ \begin{array}{l} V = -30 \text{ meV} \\ \tau = 46 \text{ meV} \end{array} \right.$$



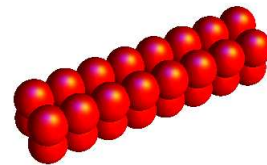
$$n_p = 1$$

$$Z = 2, Z_e = 1$$

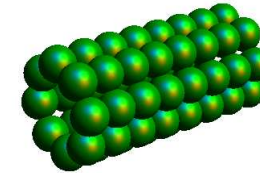


$$n_p = 2$$

$$Z = 3, Z_e = 2$$

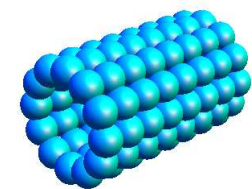


$$n_p = 4$$



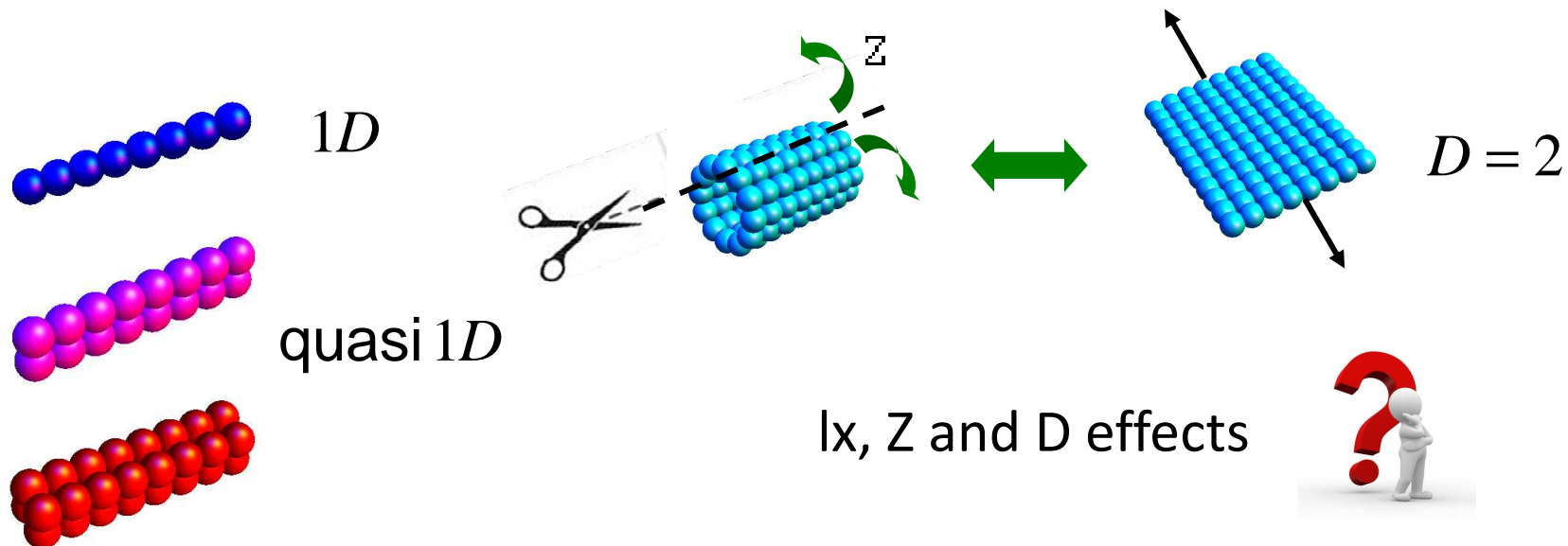
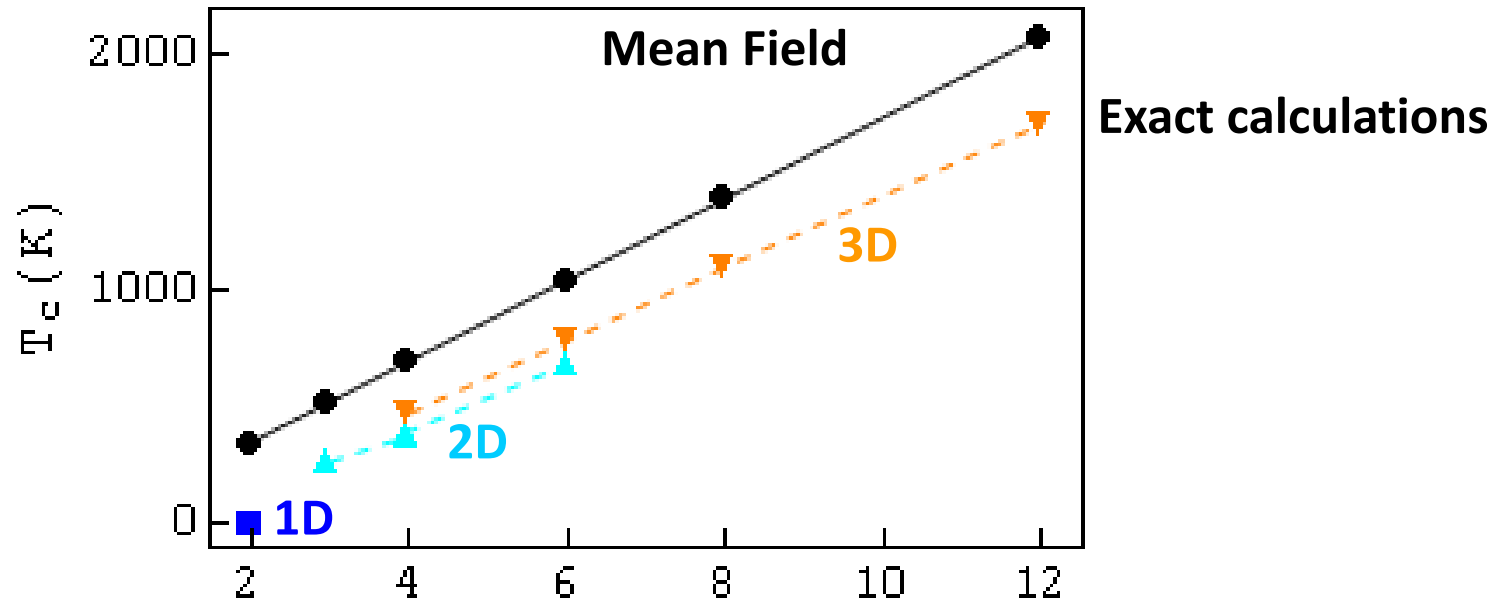
$$n_p = 8$$

$$Z = 4, Z_e = 3$$



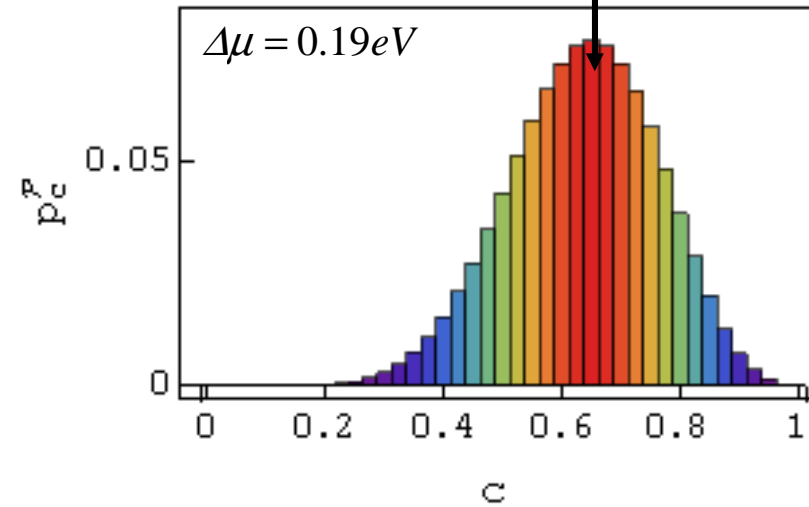
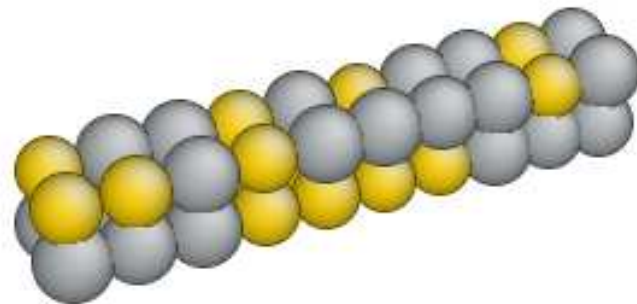
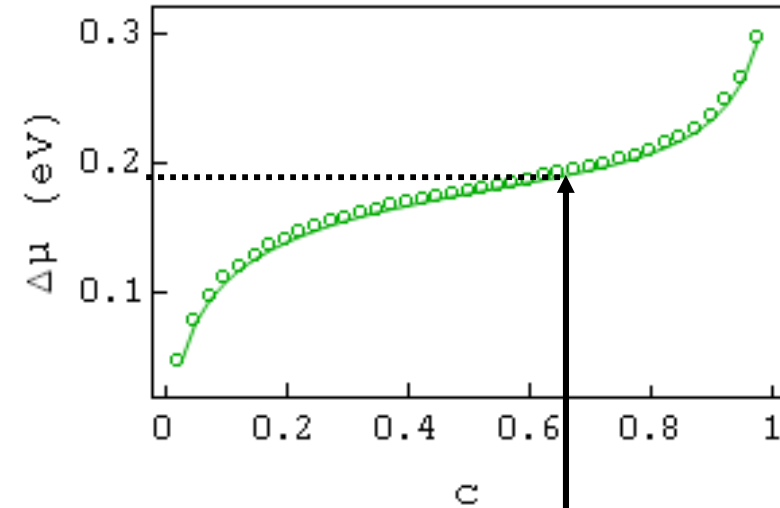
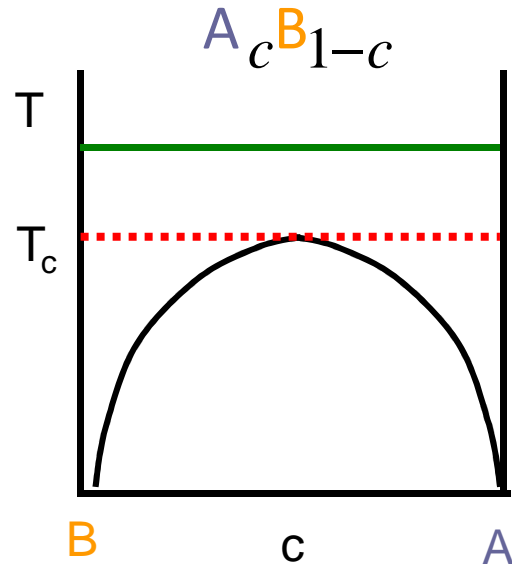
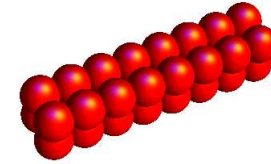
$$n_p = 12$$

Size and dimensionality effects



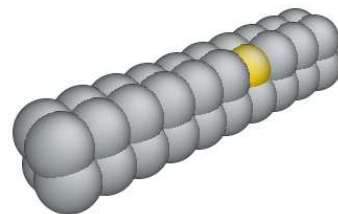
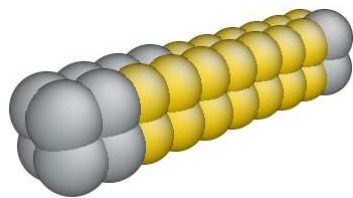
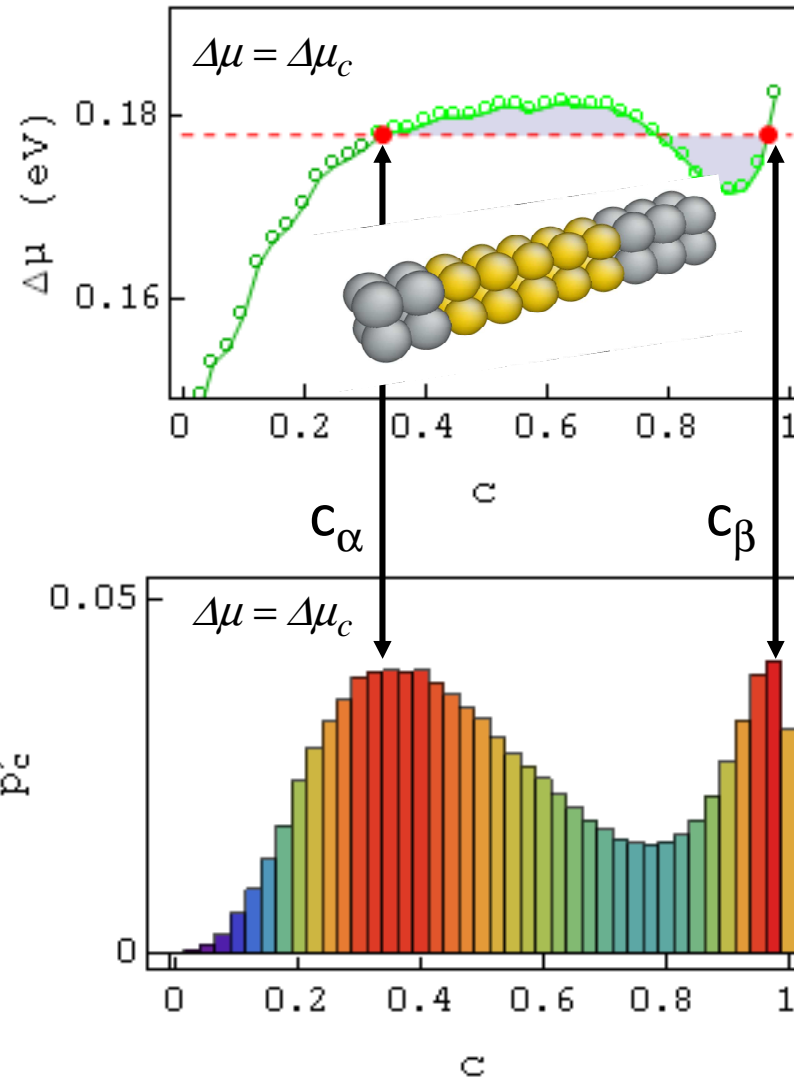
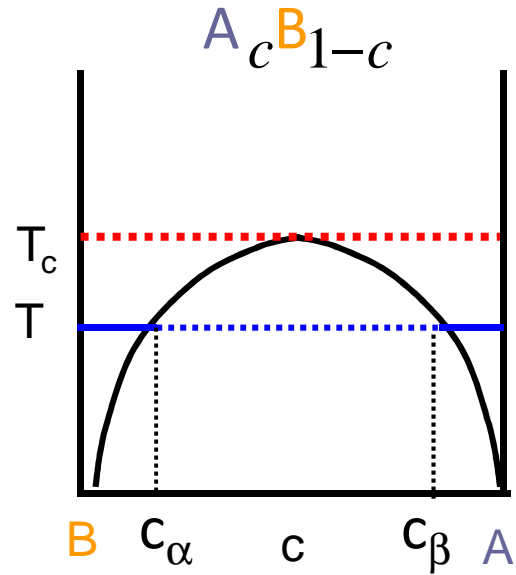
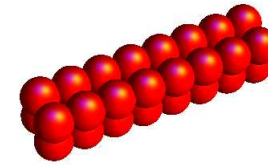
High temperature

$$T > T_c$$

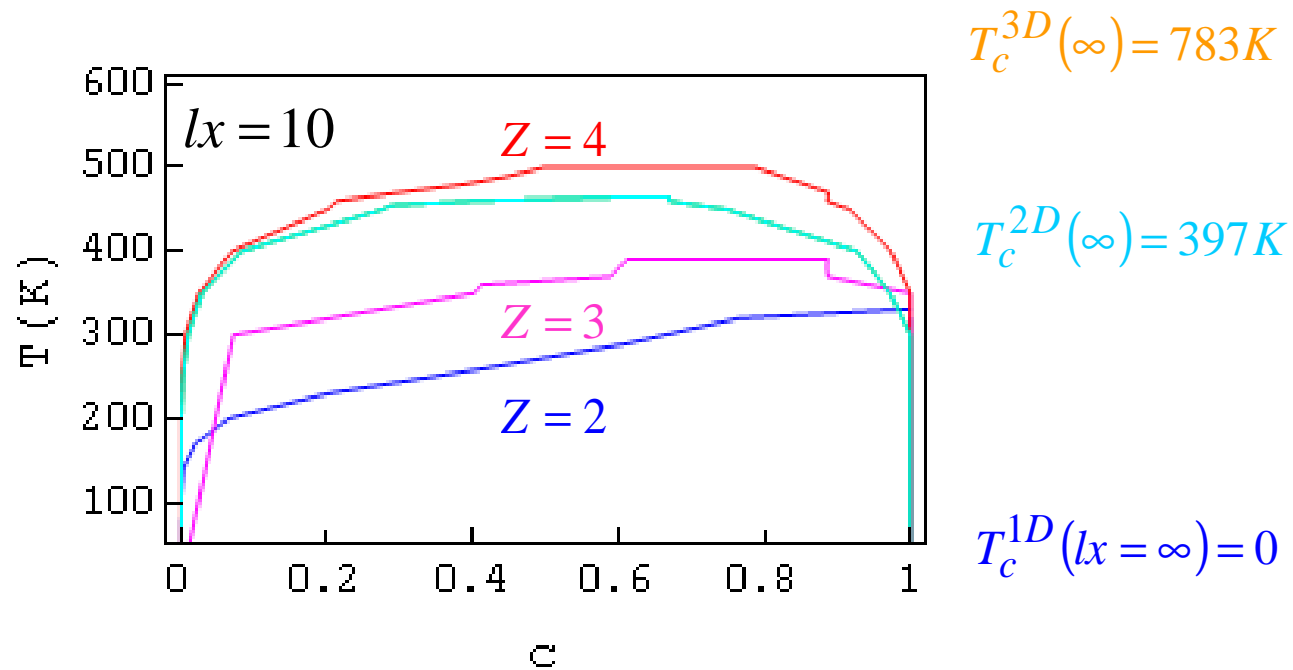


Low temperature

$$T < T_c$$



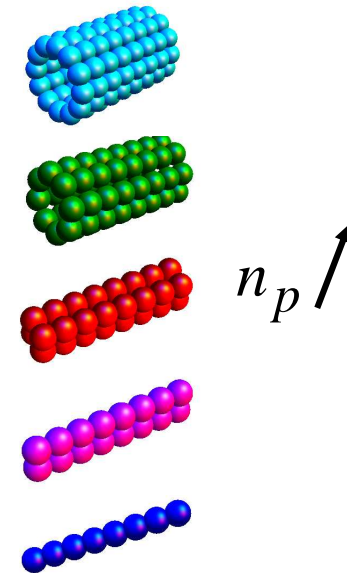
Phase Diagram



$$T_c^{3D}(\infty) = 783K$$

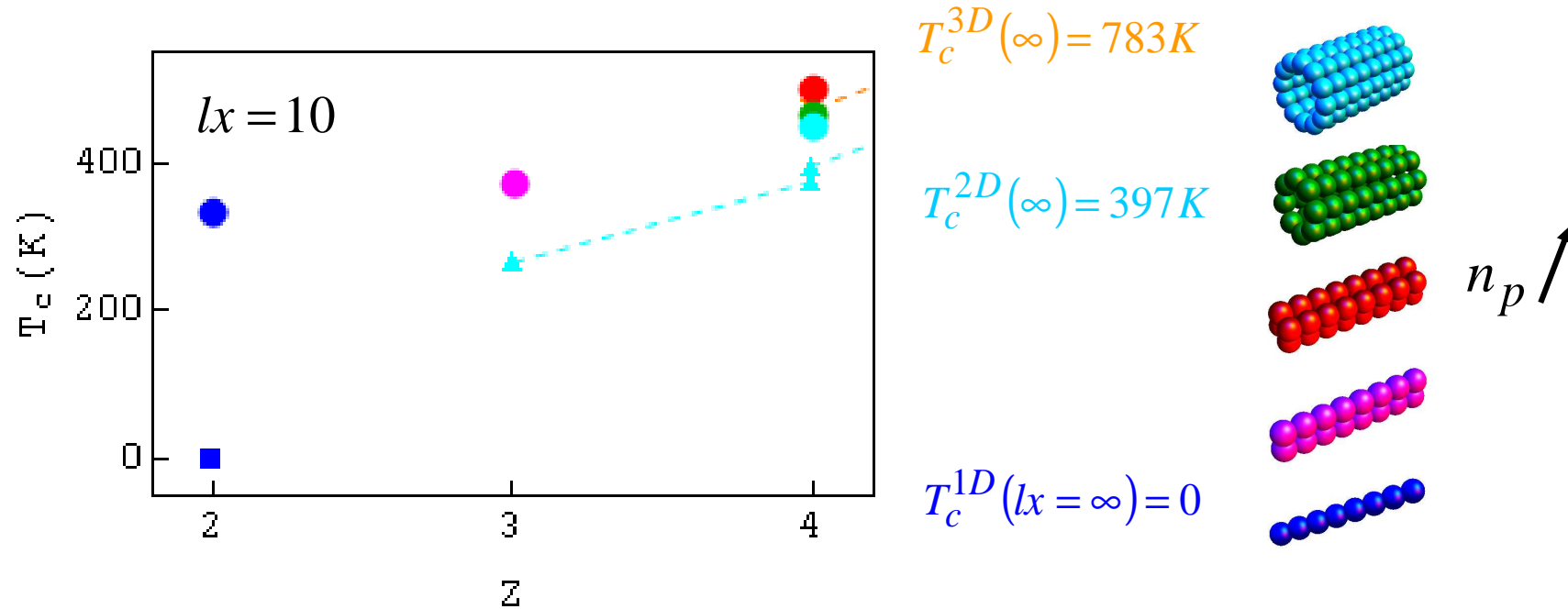
$$T_c^{2D}(\infty) = 397K$$

$$T_c^{1D}(l_x = \infty) = 0$$



$$T_c^{1D}(l_x = 10) > T_c^{1D}(l_x = \infty) = 0K!!!!$$

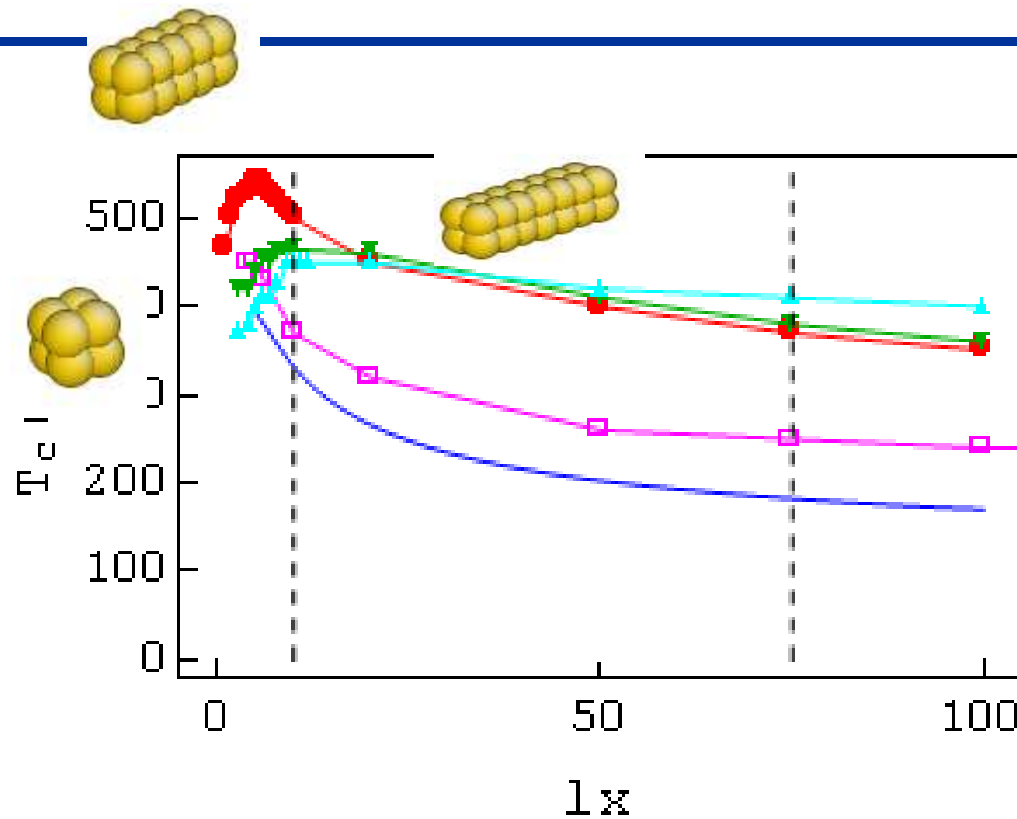
Phase Diagram



$$T_c^{2D}(l_x = 10) > T_c^{2D}(\infty)$$

T_c is increasing with increasing Z but is not % to Z

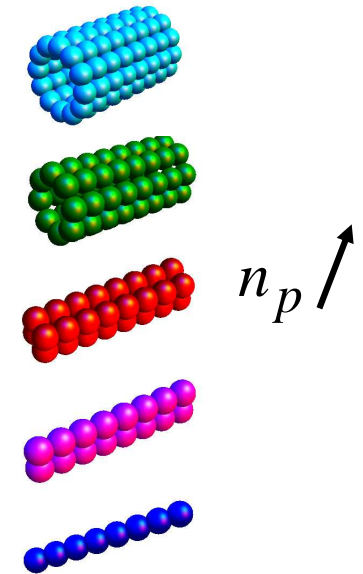
Critical temperature



$$T_c^{3D}(\infty) = 783 K$$

$$T_c^{2D}(\infty) = 397 K$$

$$T_c^{1D}(l_x = \infty) = 0$$



$$T_c^{2D}(l_x) > T_c^{2D}(\infty)$$

Z=4 : Non monotonous variation of T_c with l_x

Z=4 : T_c decreases (increases) with increasing n_p for $l_x < 25$ ($l_x > 25$)