



energie atomique • energies alternatives



Comprendre le monde,
construire l'avenir®

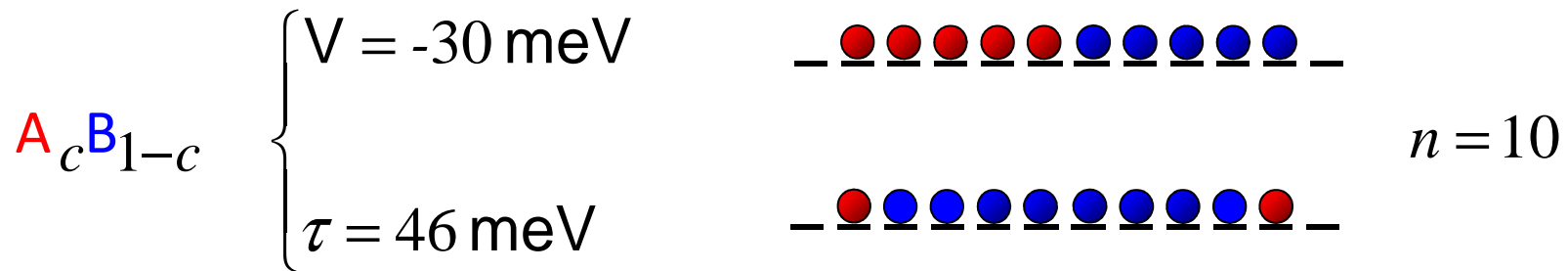
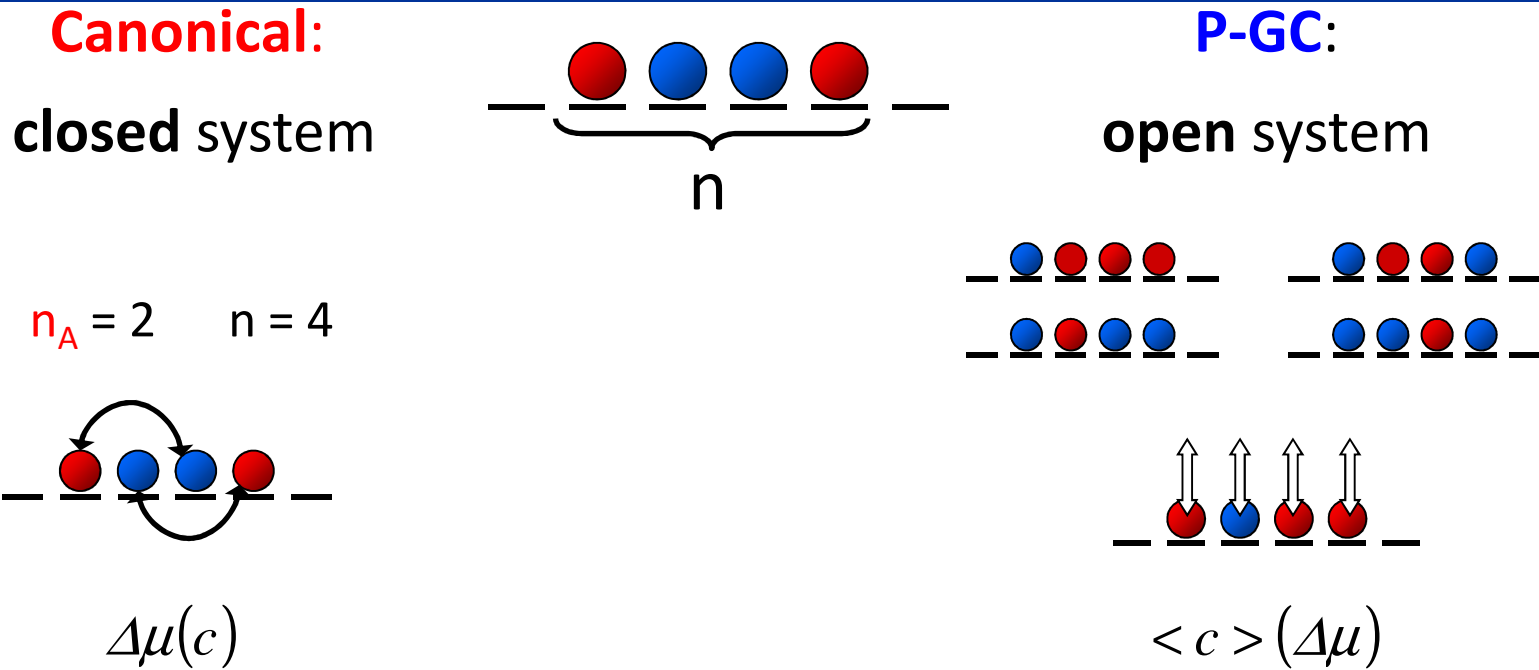
(In)equivalence of thermodynamic ensembles in bimetallic nanowires



E. Maras, F. Berthier, I. Braems, B. Legrand

EMCMRE-2

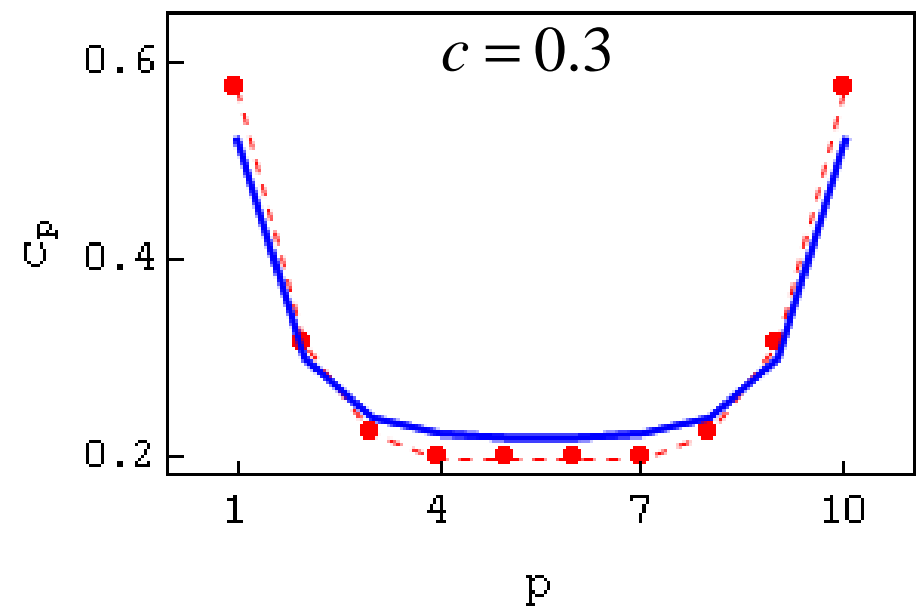
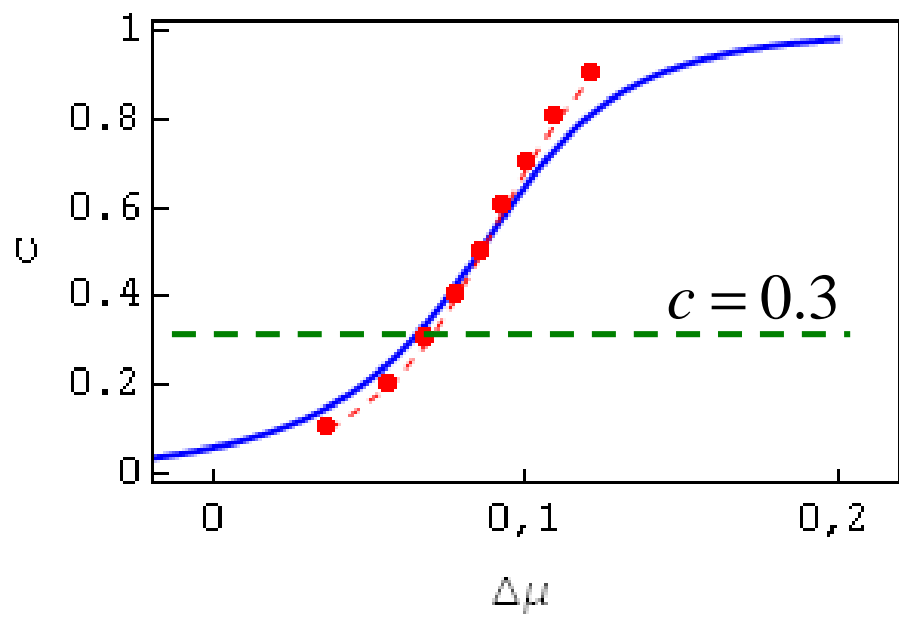
From one nanowire... to nanowire_S



Monte Carlo simulations

Comparison at $T = 500$ K

● Canonical
— P-GC

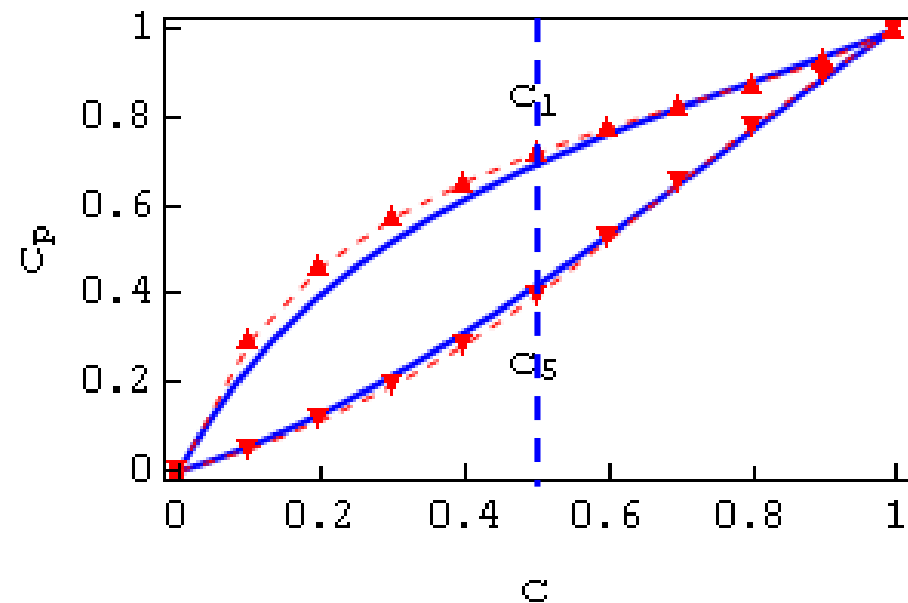
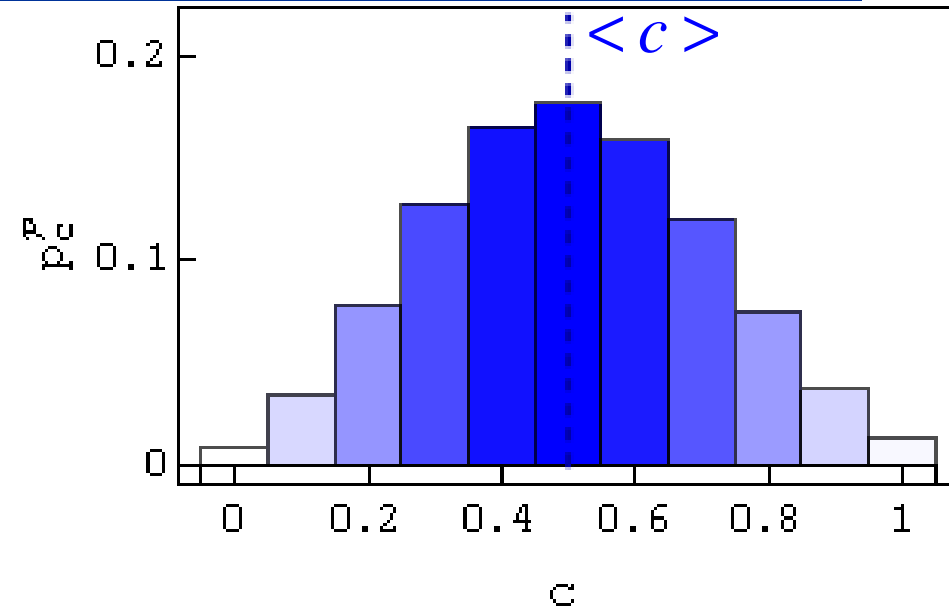
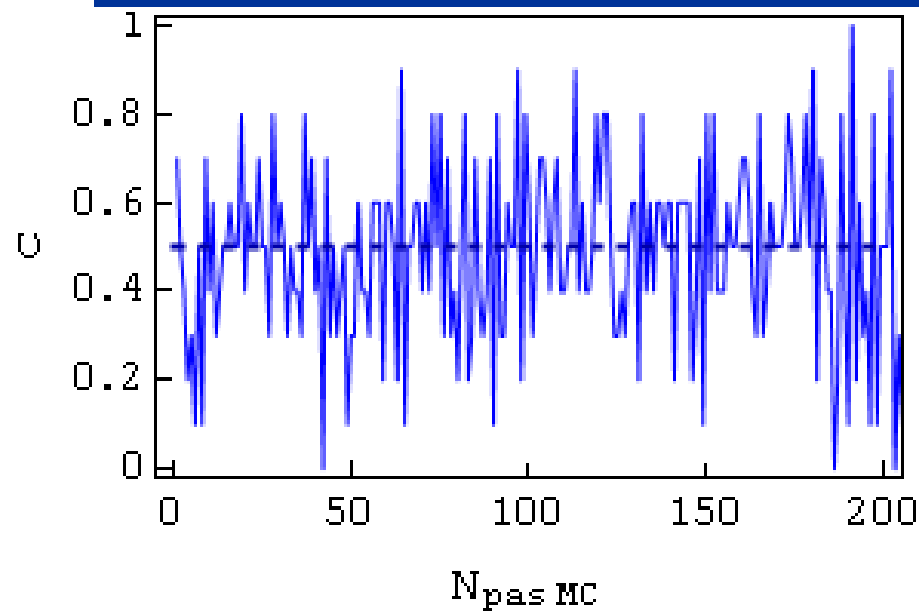


Canonical isotherm
is steeper

Canonical segregation
is stronger

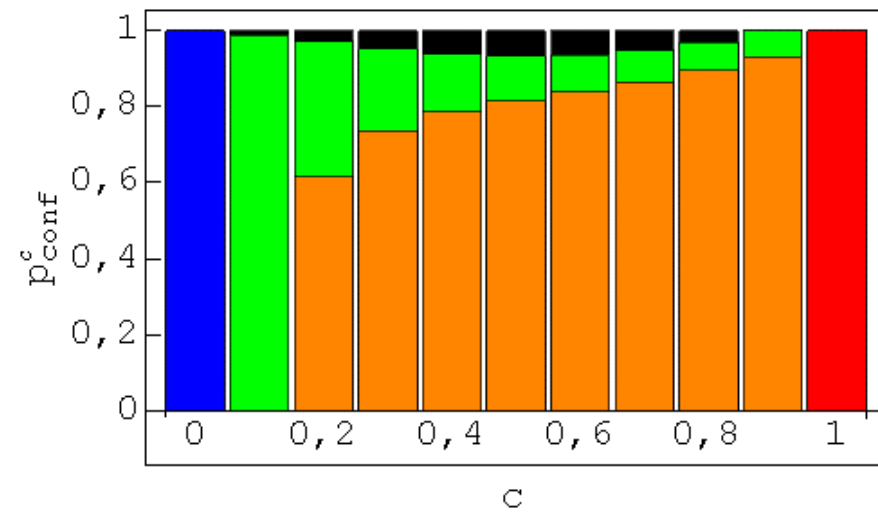
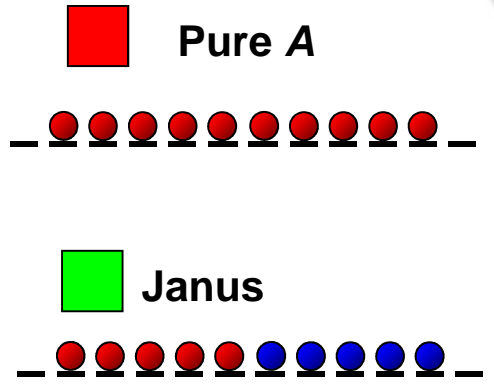
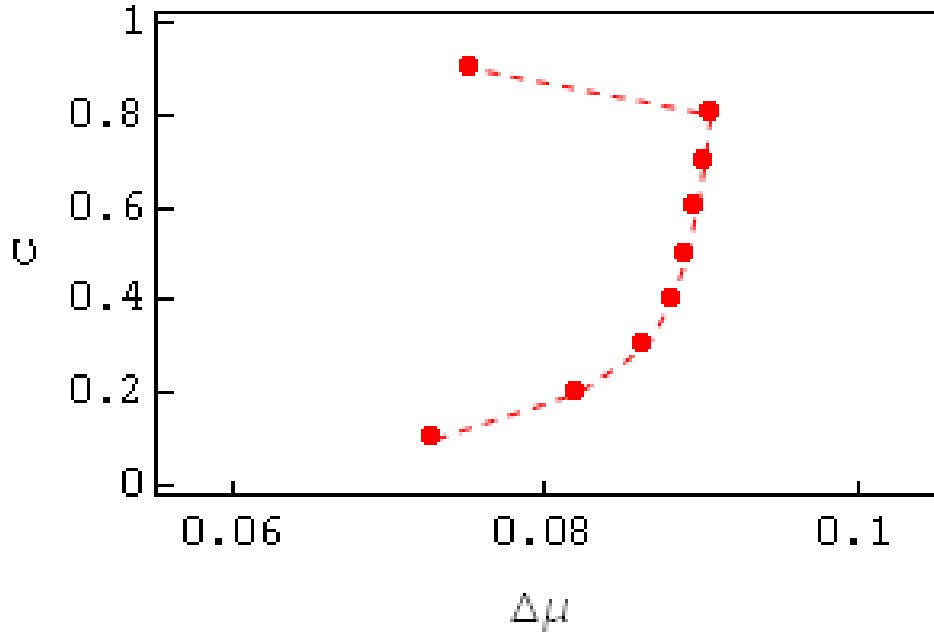
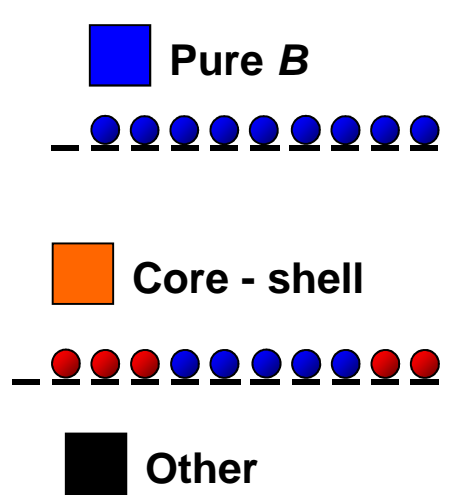
Even at high temperature the two ensembles are not equivalent for small systems

Link between P-GC and Canonical ensembles

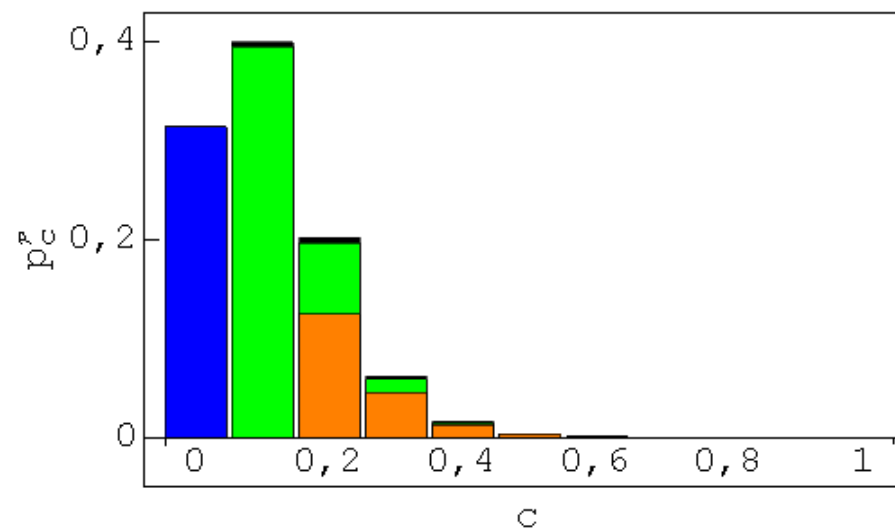
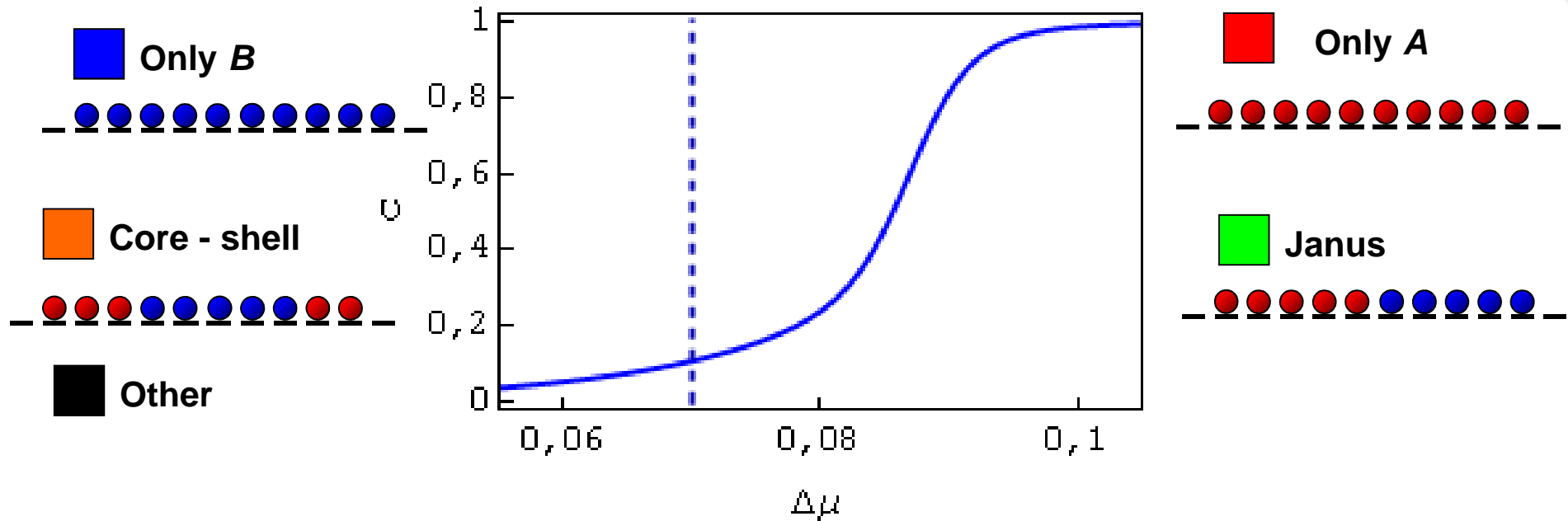


$$f_{\langle c \rangle}^P = \sum_c f^C(c) P_c^P(\langle c \rangle)$$

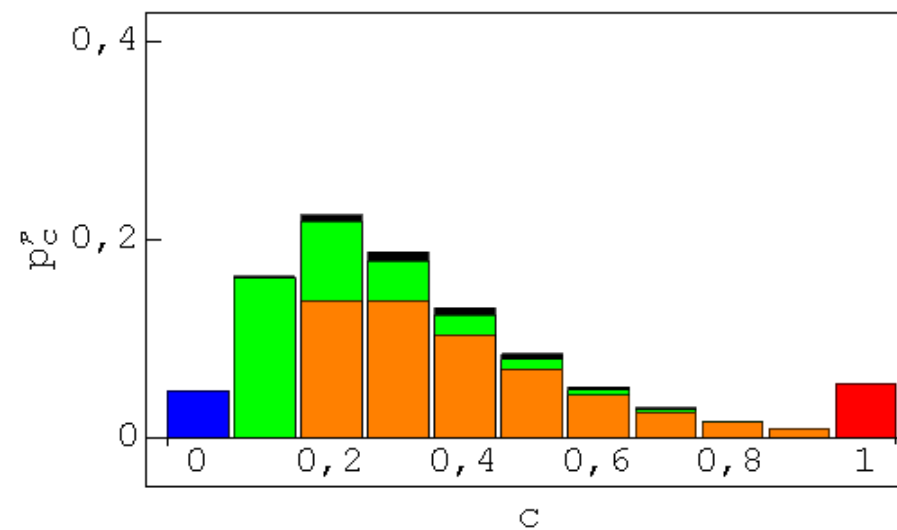
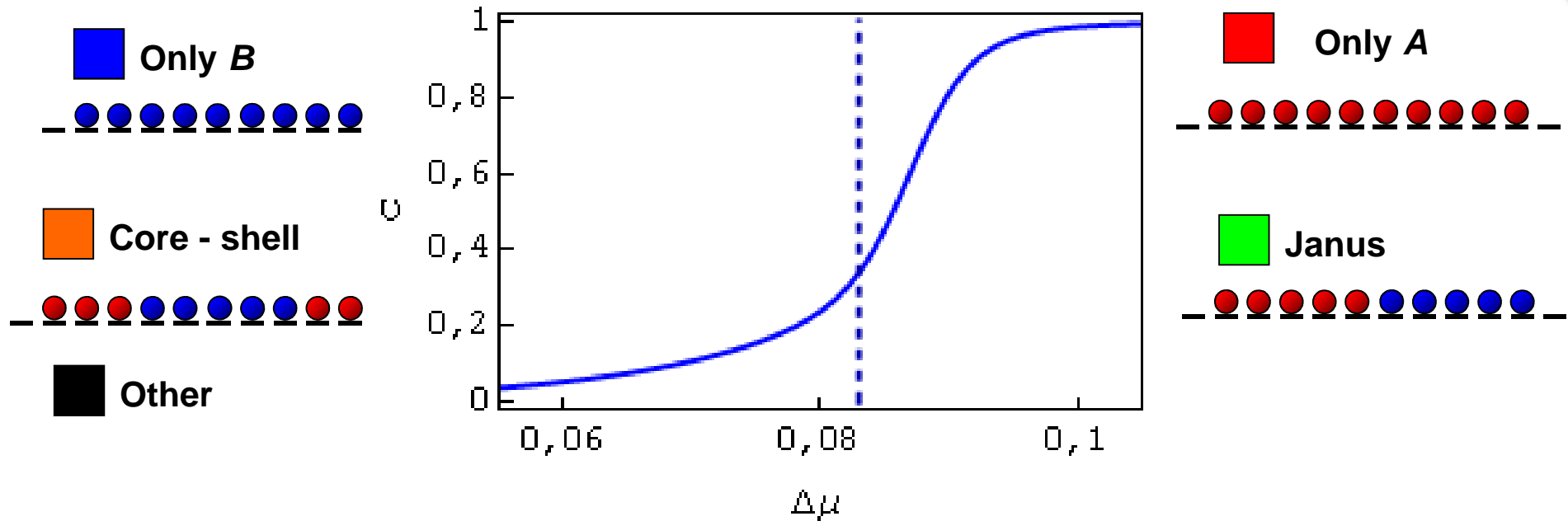
Canonical isotherm and configurations at $T = 150\text{ K}$



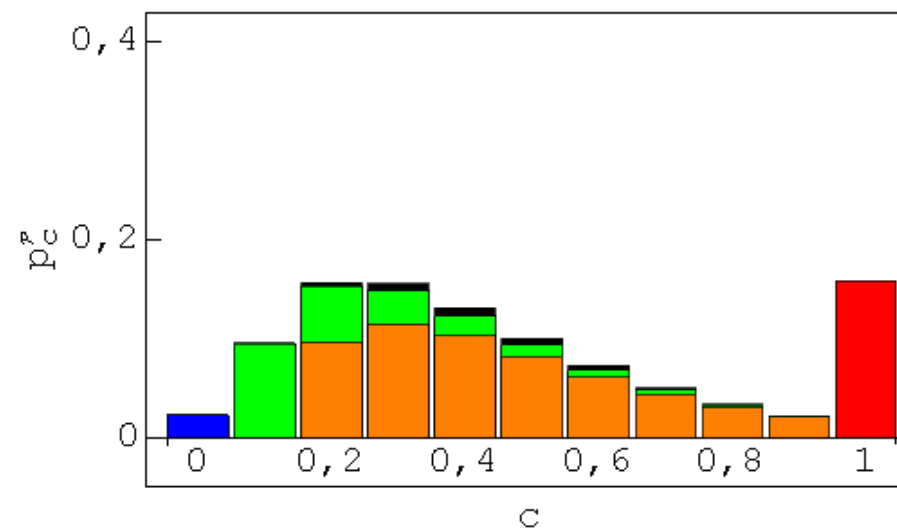
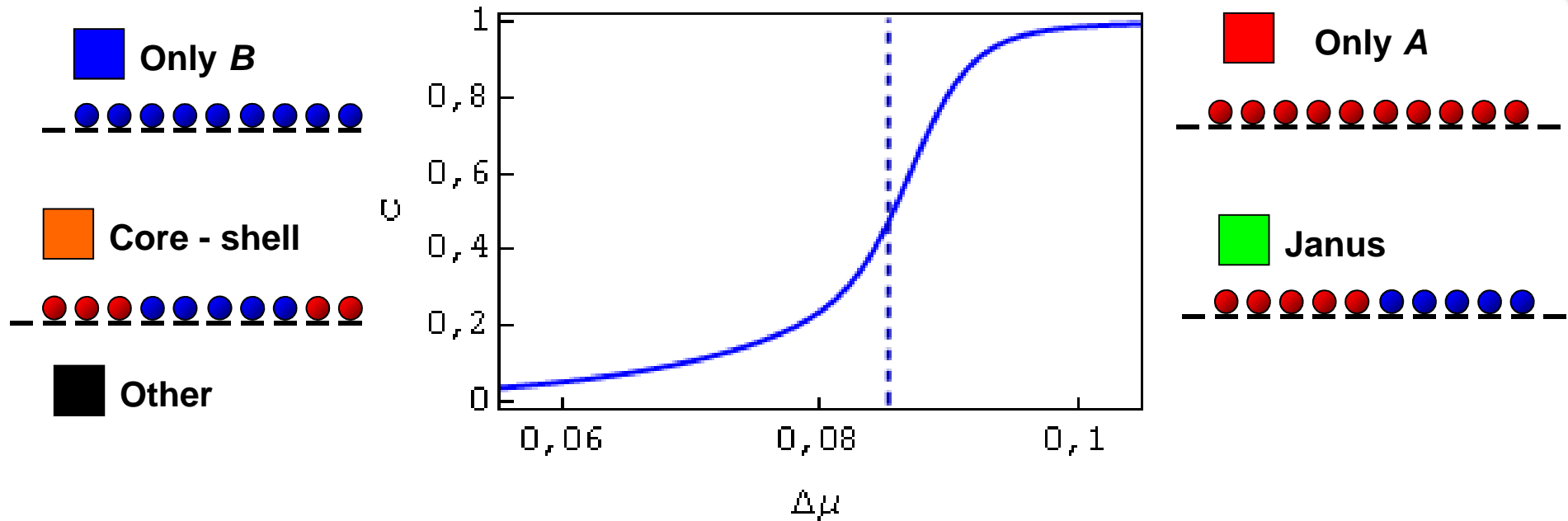
P-GC isotherm and configurations at $T = 150 \text{ K}$



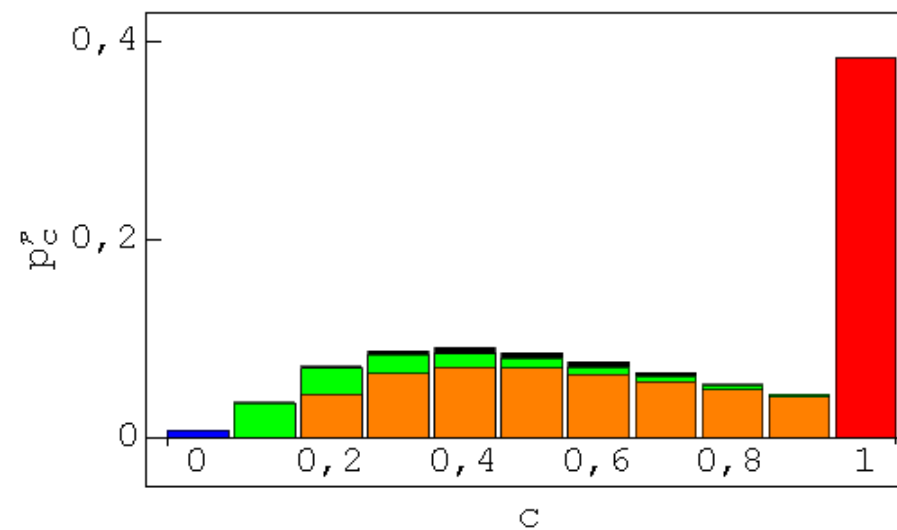
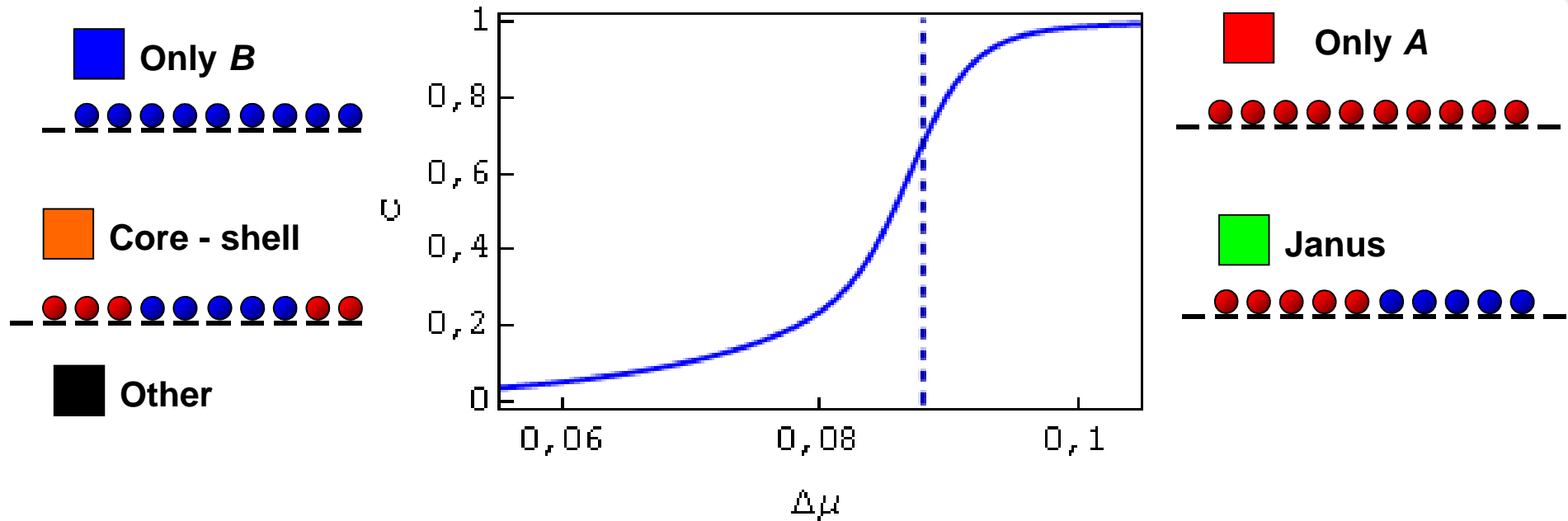
P-GC isotherm and configurations at $T = 150$ K



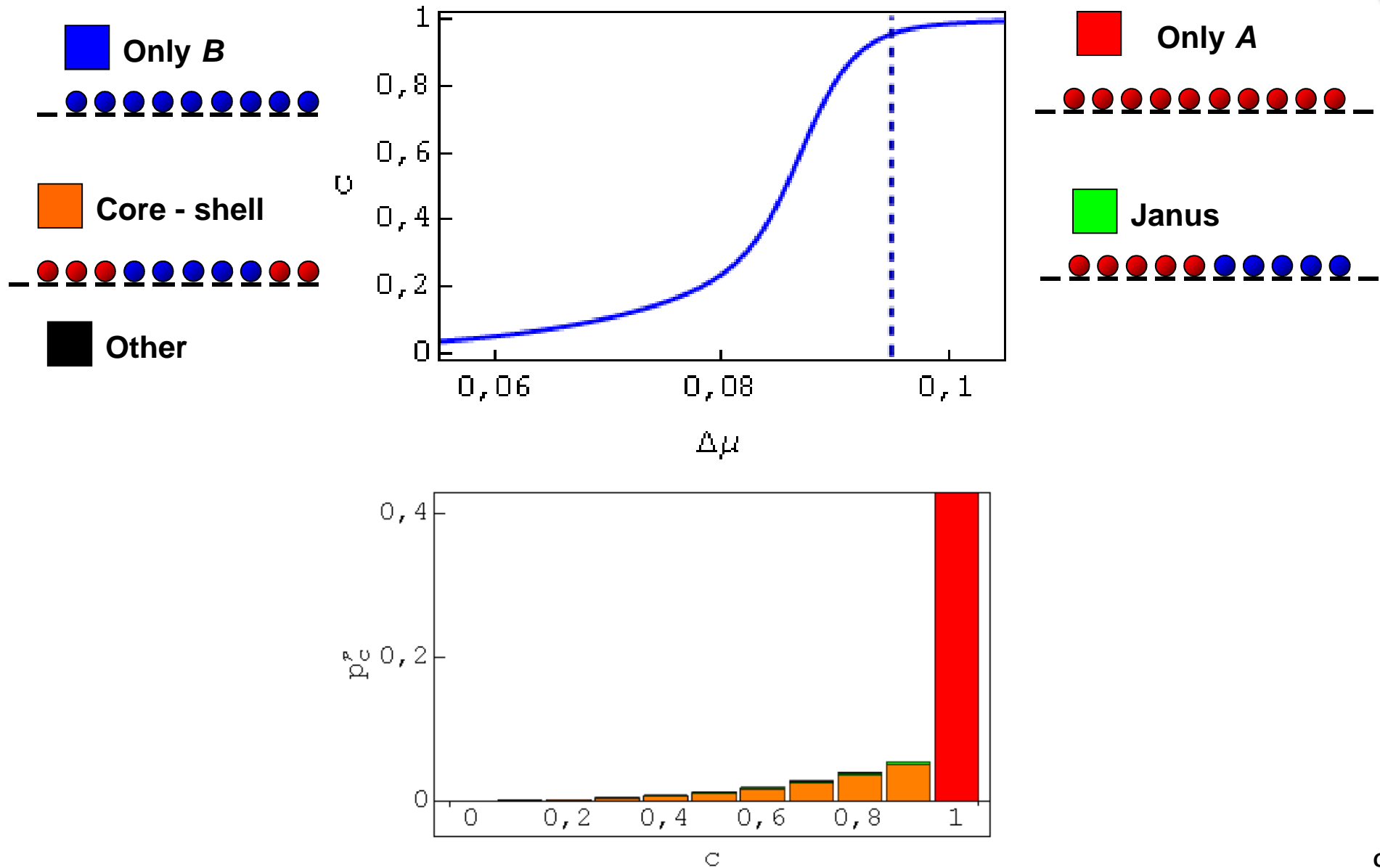
P-GC isotherm and configurations at $T = 150$ K



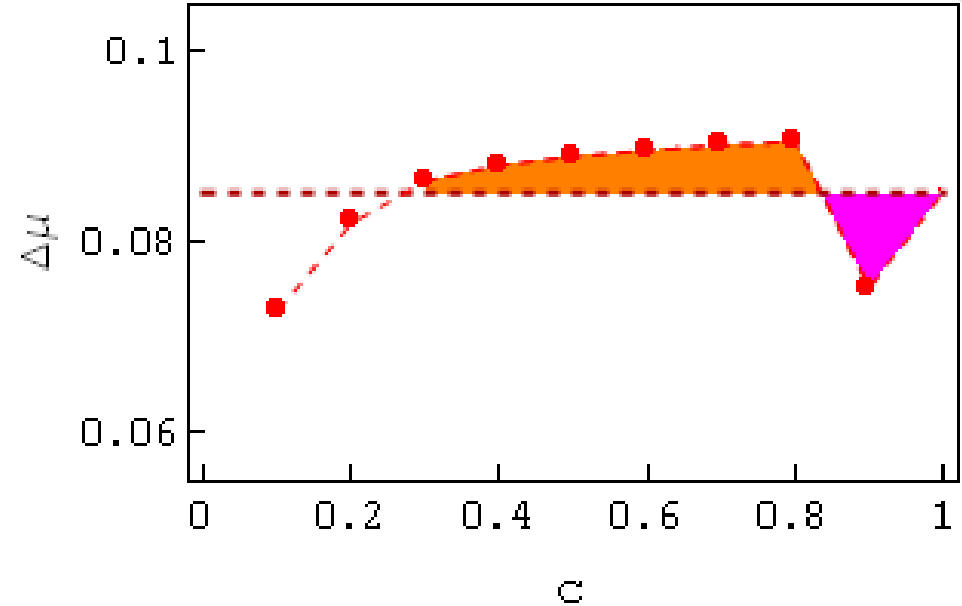
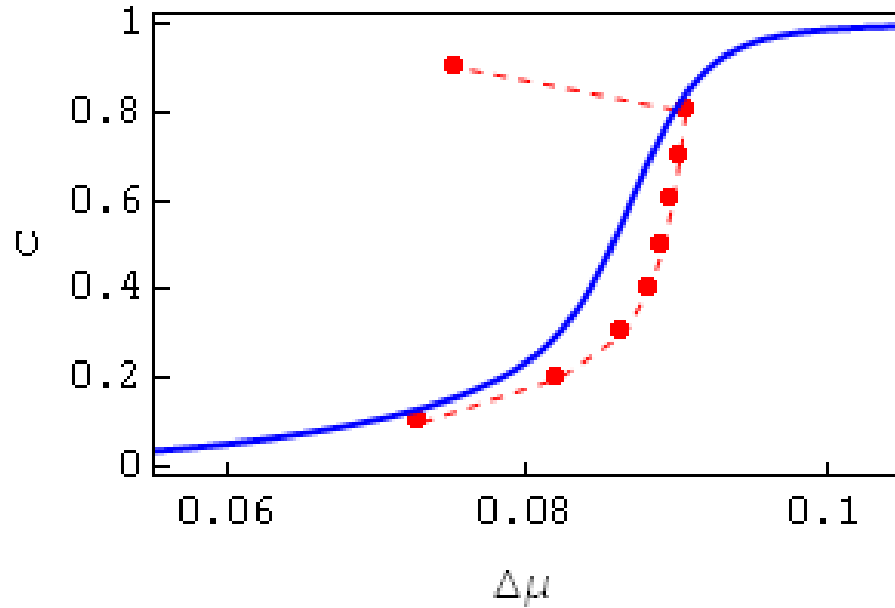
P-GC isotherm and configurations at $T = 150$ K



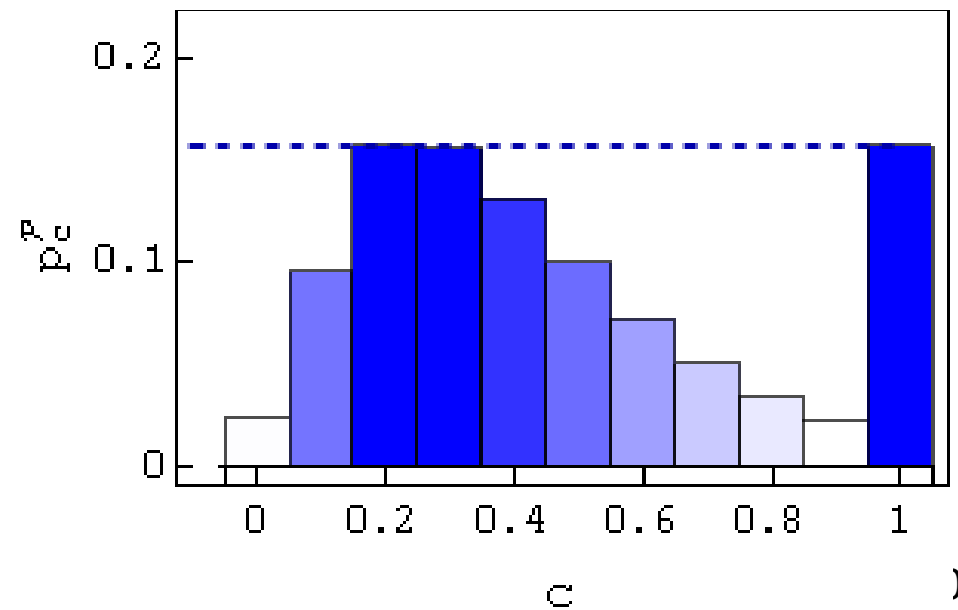
P-GC isotherm and configurations at $T = 150 \text{ K}$



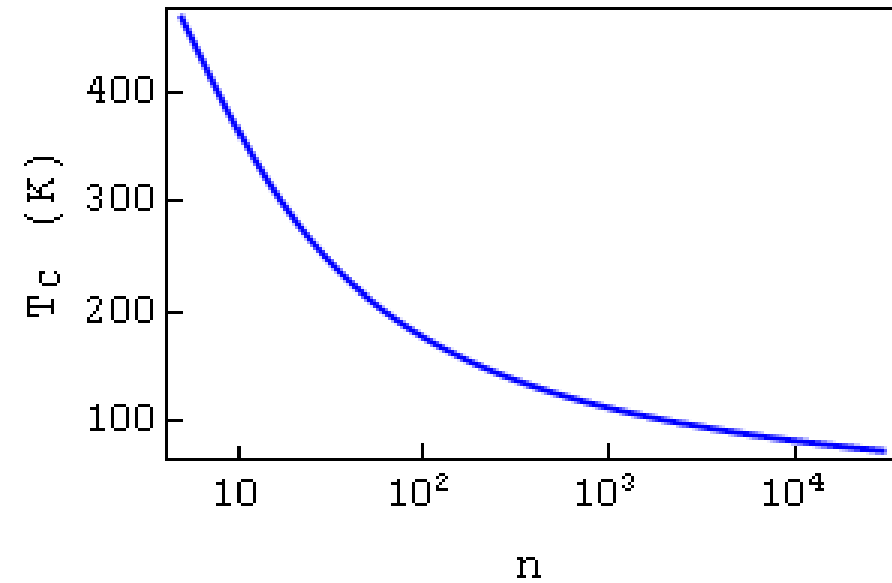
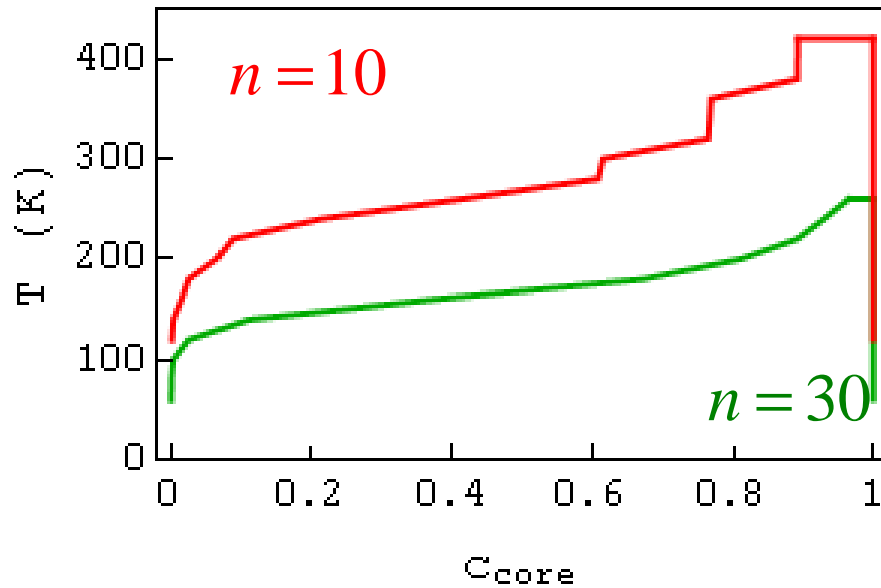
Comparison at $T = 150\text{ K}$



Signature of phase transition



Phase Diagram



Chains... Nanowires...Nanotubes

