A novel ground state of KOs_2O_6 lattice?

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Why AOs_2O_6?

- Physics on the triangular lattice:

  superconductivity - $LiTi_2O_4$, LiV_2O_4, $Na_xCoO_2.H_2O$, $Cd_2Re_2O_7$;

  charge ordering - $CuIr_2S_4$, $Tl_2Ru_2O_7$
- KOs_2O_6 vs $RbOs_2O_6$, $CsOs_2O_6$ - isoelectronic materials with surprisingly different physical properties (superconductivity, transport and low temperature thermodynamics)

Why?

Superconductivity

	a (Å)	T_c (K)
KOs_2O_6	10.101	9.6
$RbOs_2O_6$	10.114	6.3
$CsOs_2O_6$	10.149	3.2

KOSO - non-s-wave pairing (T_1 NMR, muons), H_{c2} above Pauli limit
ROSO,COSO - BCS type superconductivity
Superconductivity suppressed by pressure ~ 5 GPa (suppression of $N(E_F)$ - Saniz private commun.)

Hiroi *et al*. J. Phys. Soc. Jpn. **73** 1651 (2004)

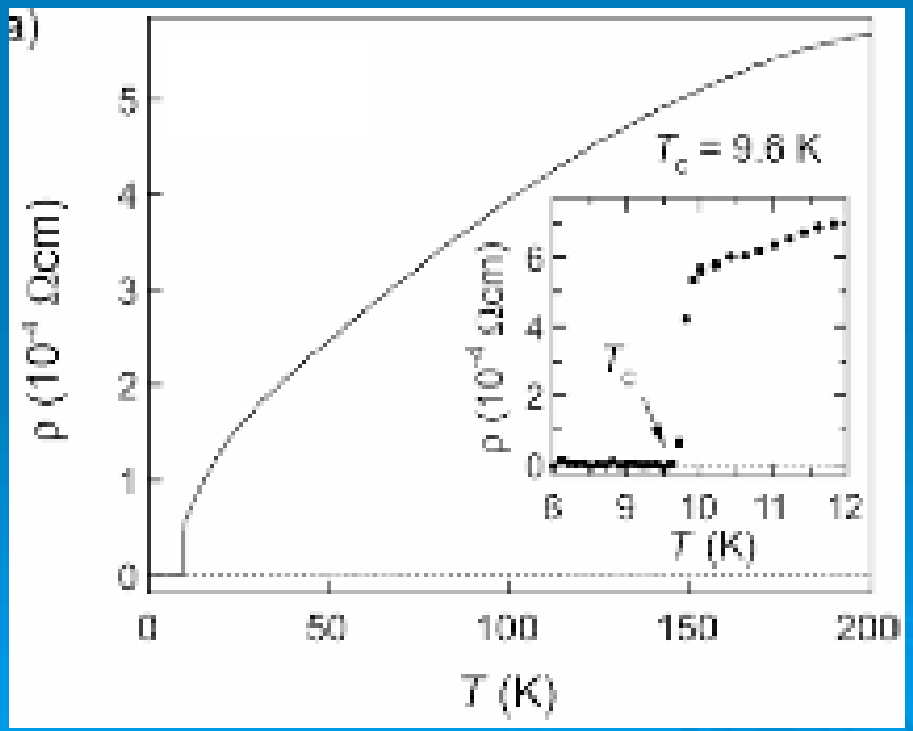
Yonezawa *et al*. J. Phys.Soc. Jpn. **73** 819 (2004), cond-mat/0404220

Muramatsu *et al*. cond-mat/0407610

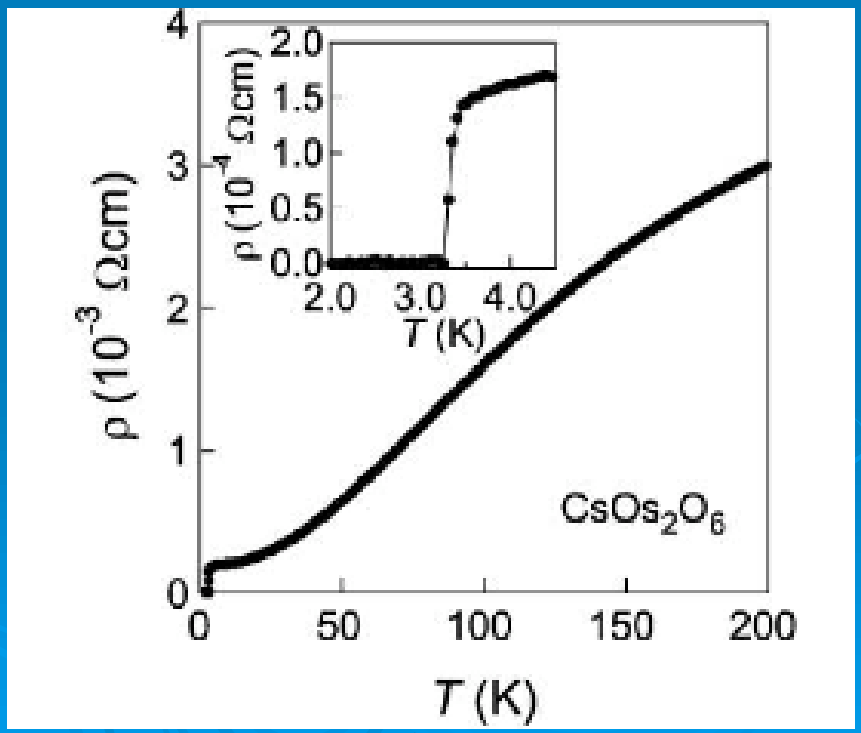
Conductivity

KOSO - non-Fermi liquid behavior vs. FL behavior in ROSO and COSO

KOs_2O_6



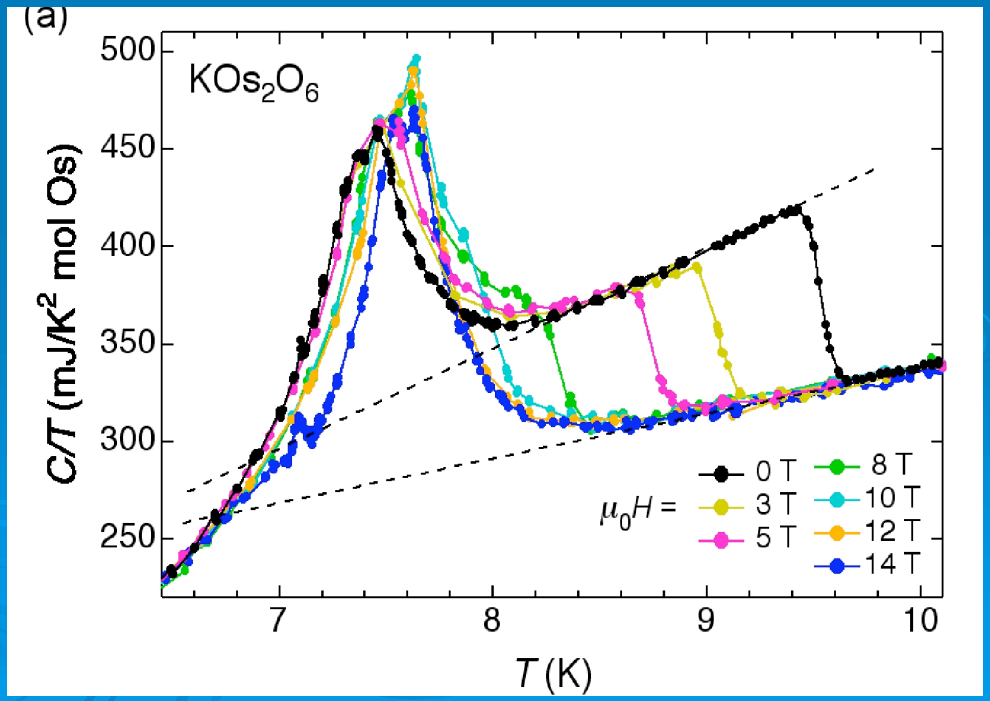
$CsOs_2O_6$



Specific heat

- Large enhancement of linear specific heat coefficient (λ~4 ROSO, COSO; λ~12 KOSO)
  - Einstein modes identified in ROSO, COSO
  - Large D-W factors associated with A
  - Second peak in KOSO :

Z. Hiroi *et al.* cond-mat/0502043



Lattice structure

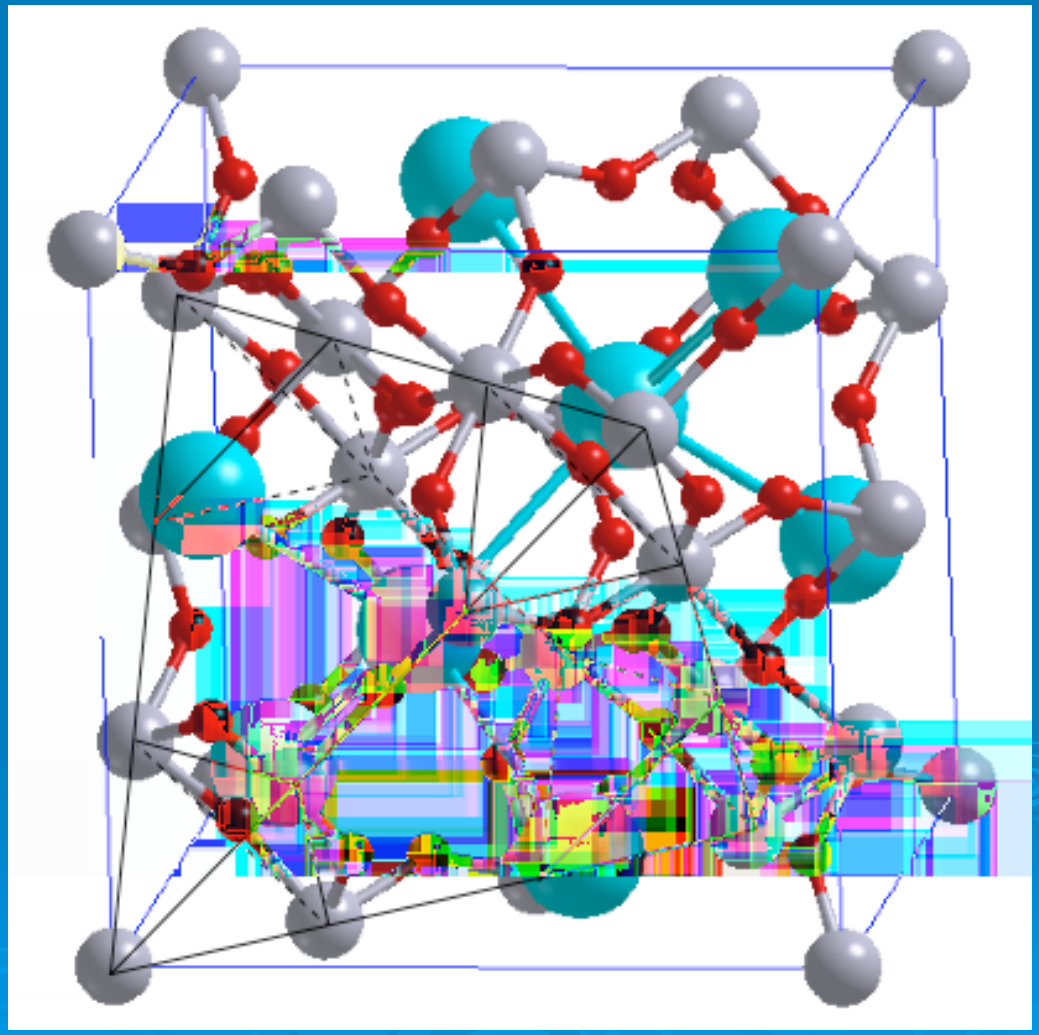
O: Os-O-Os bonds

Os: OsO_6 octahedra

Os pyrochlore lattice

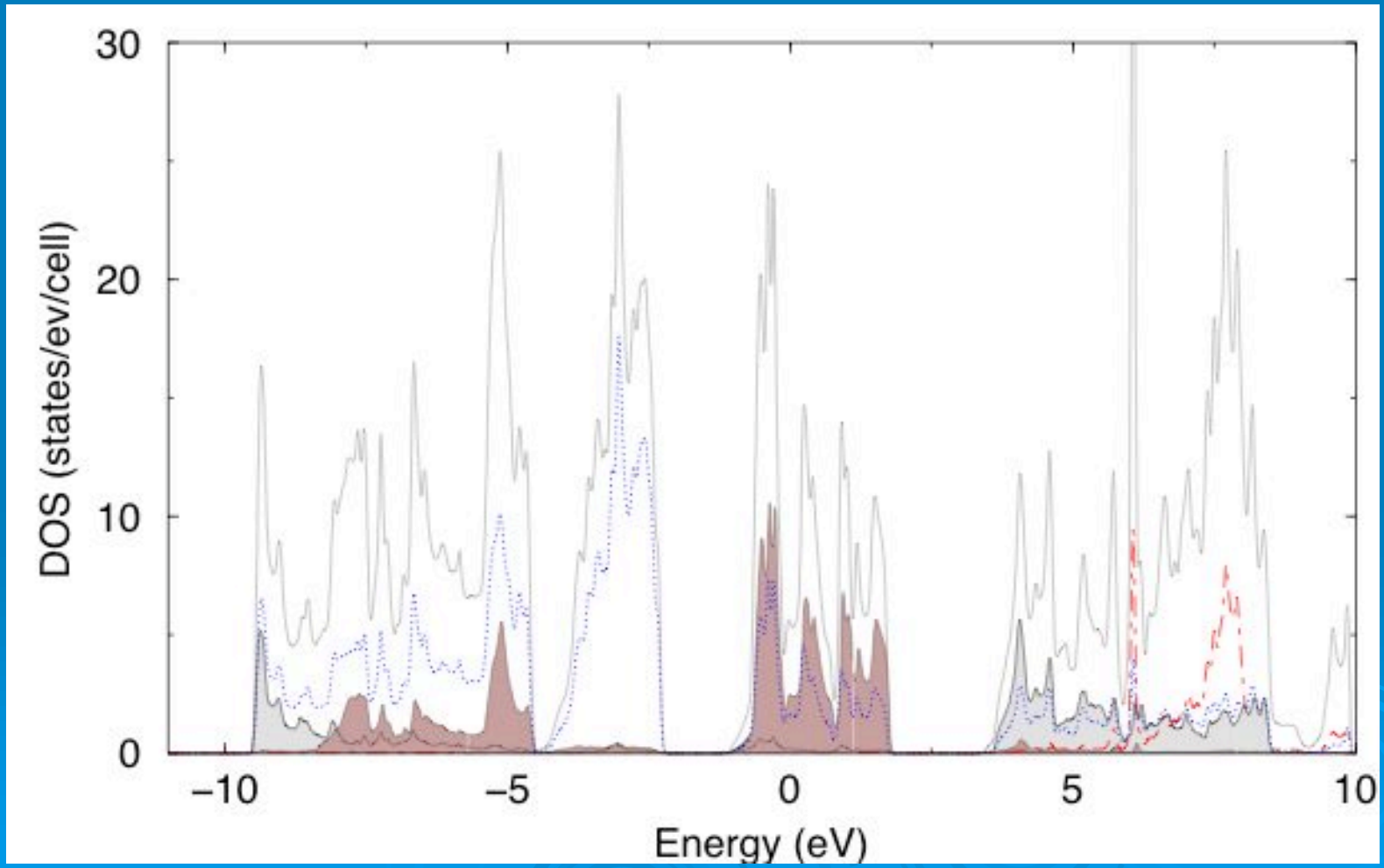
A: cavities inside the pyrochlore cage

A - diamond lattice



Density of states

Formal valency: $A^{+}Os_2^{5.5+}O_6^{2-}$ ==> $d^{2.5}$



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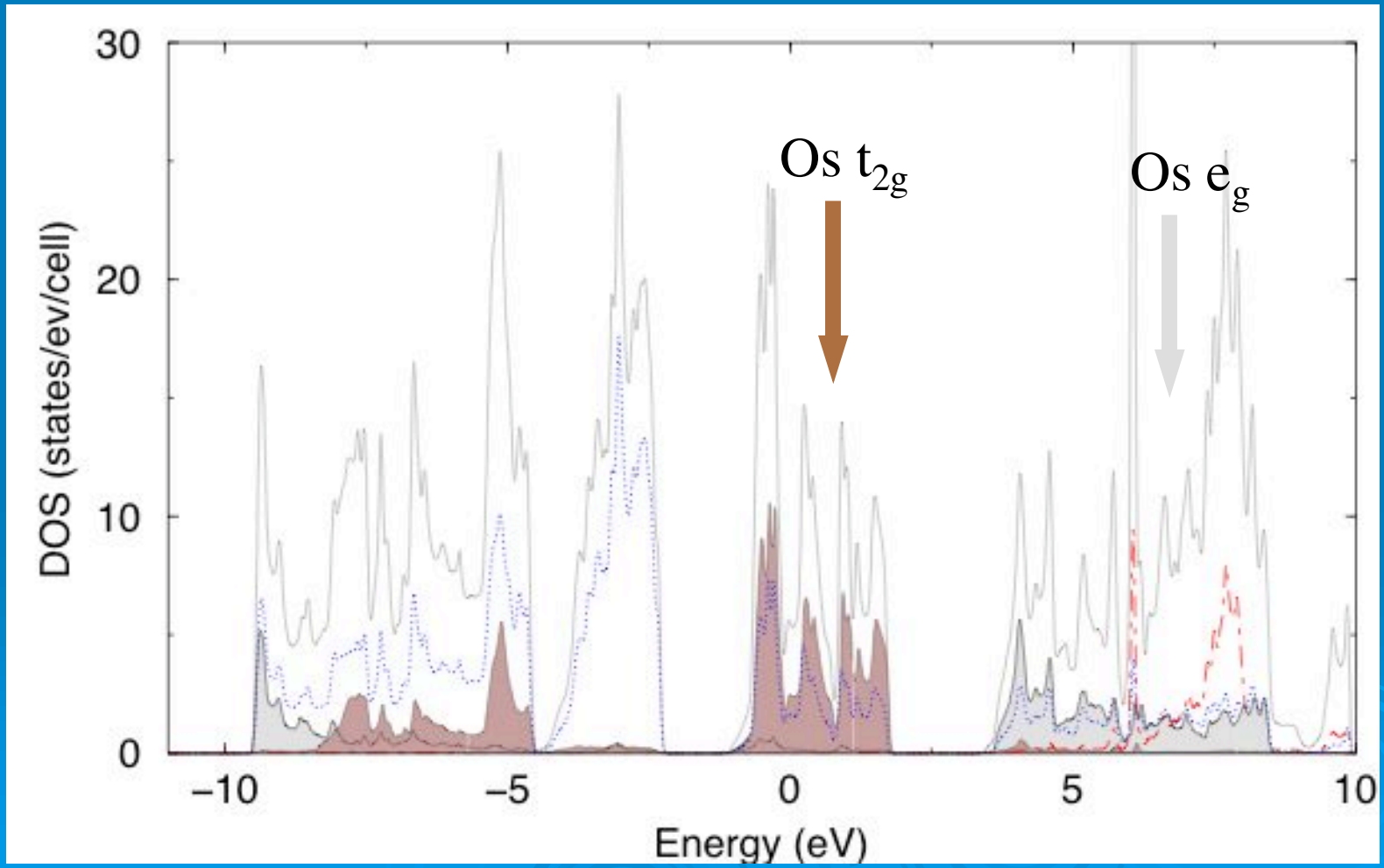

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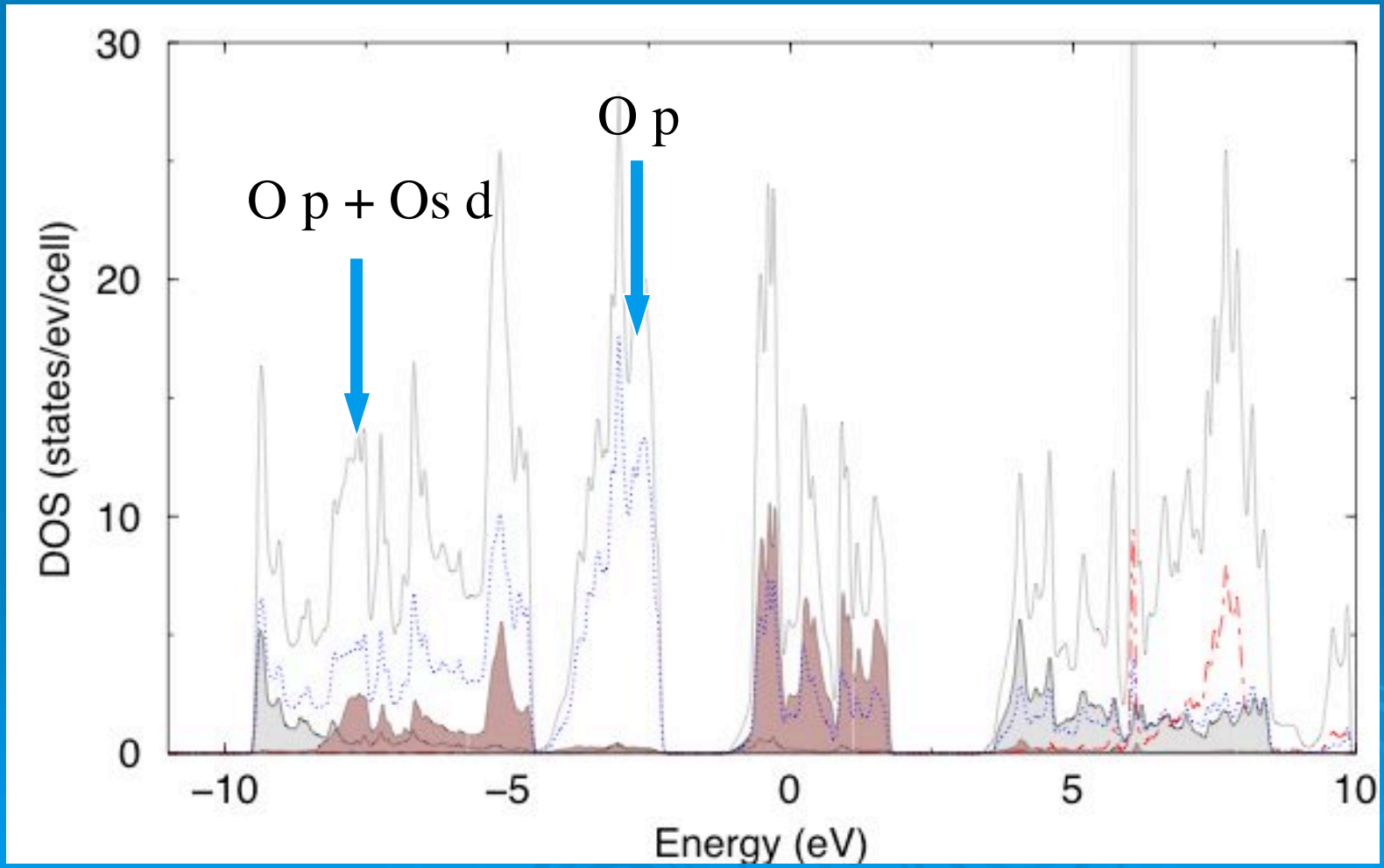

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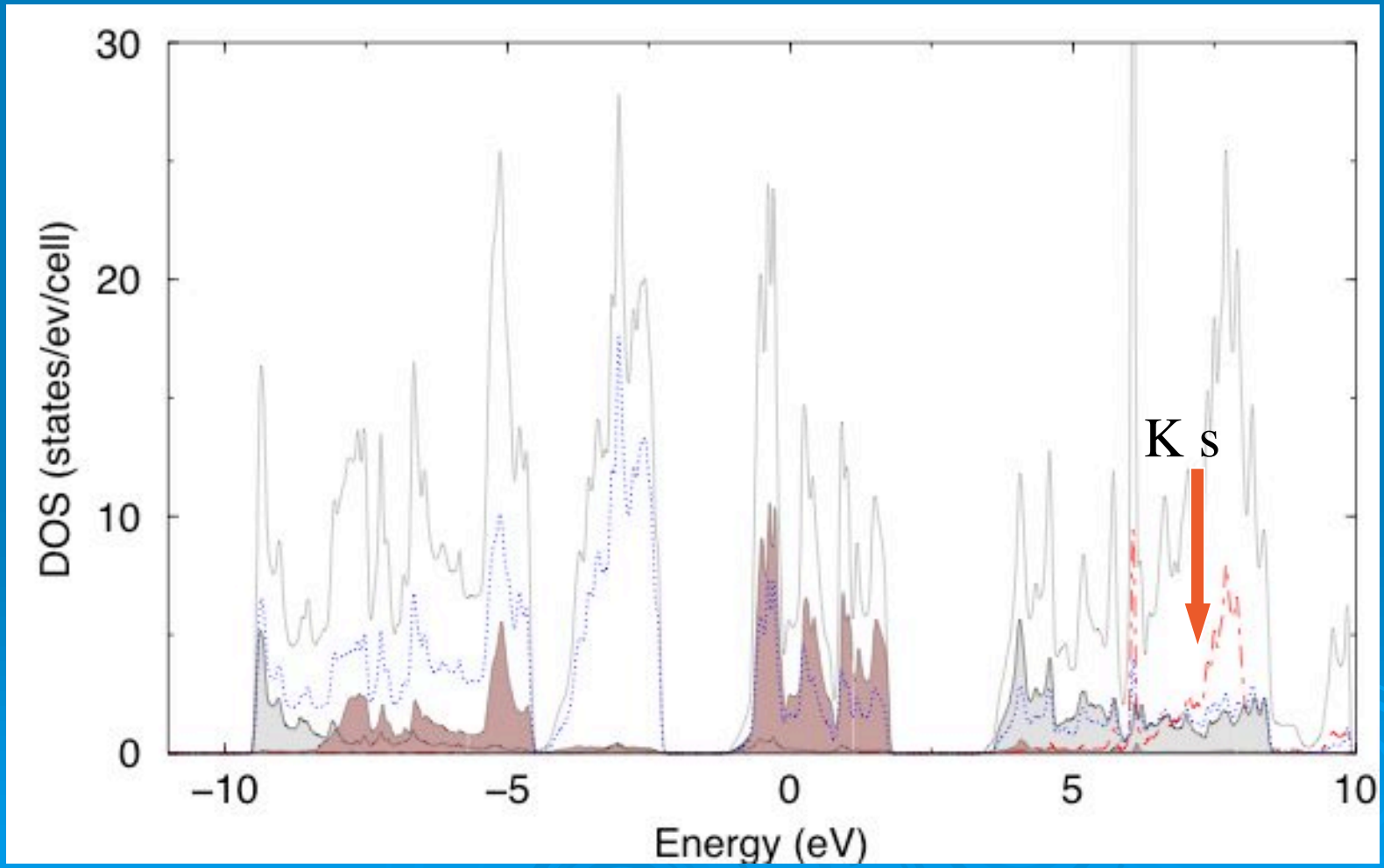
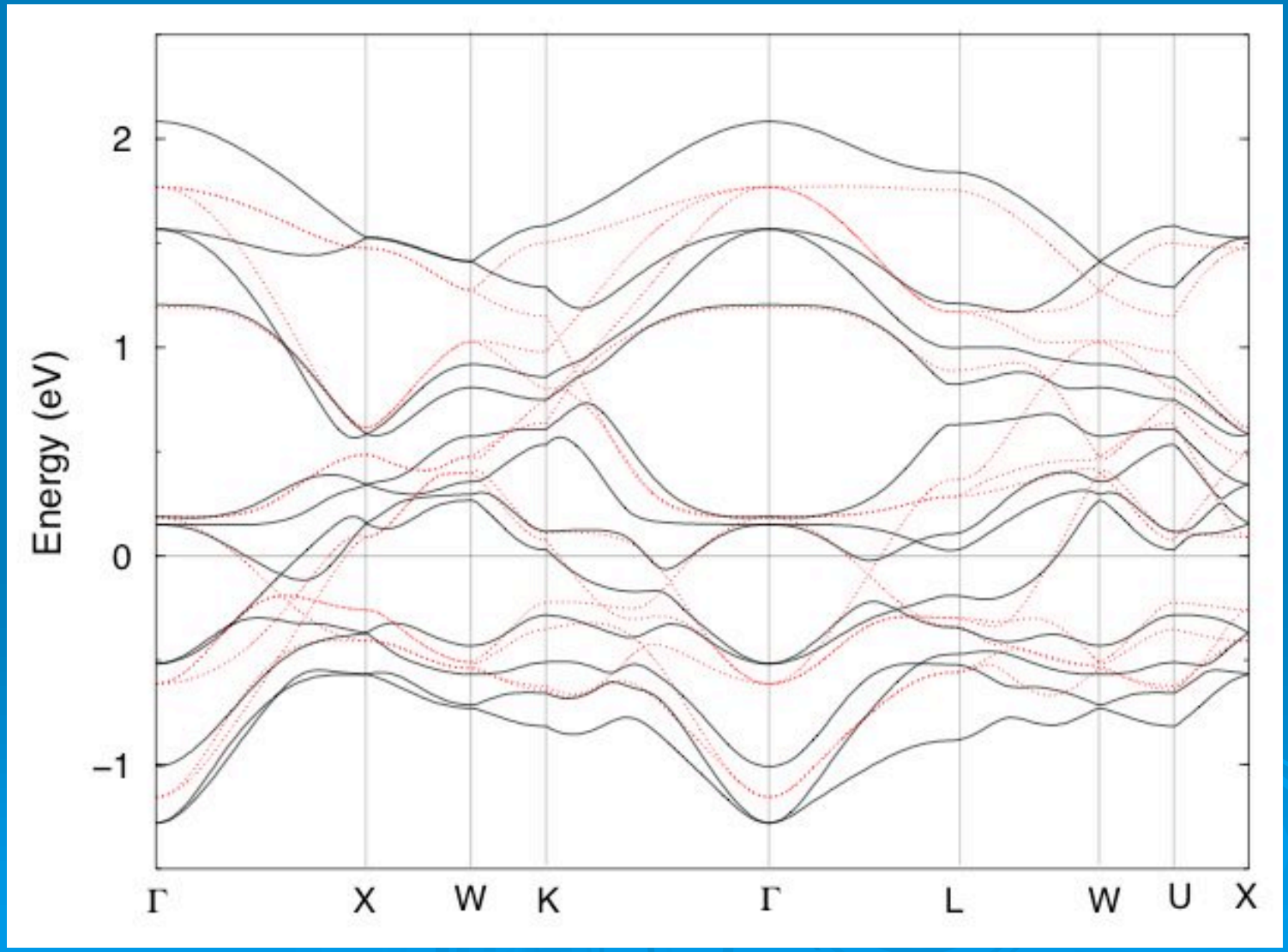
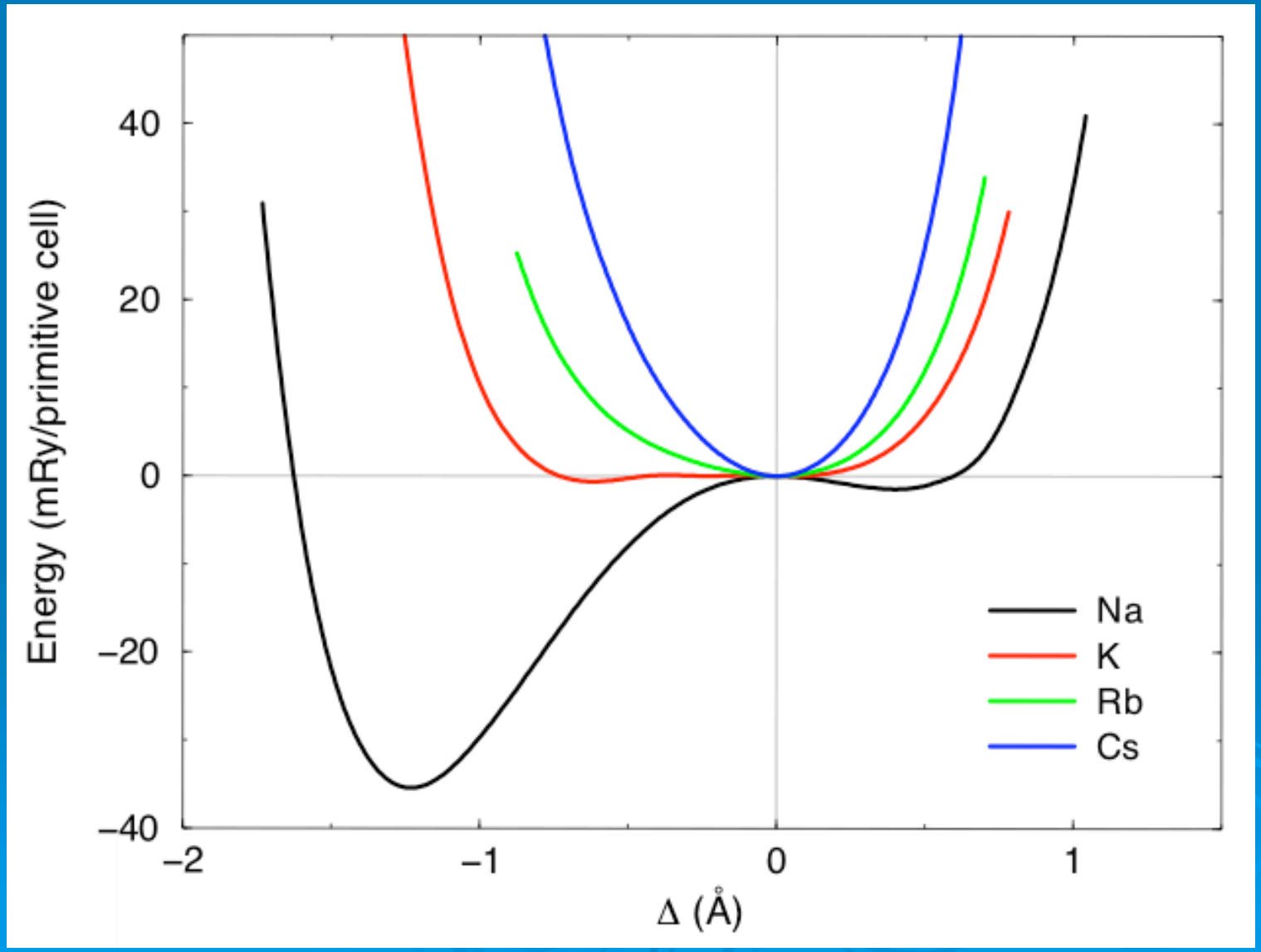


Bandstructure



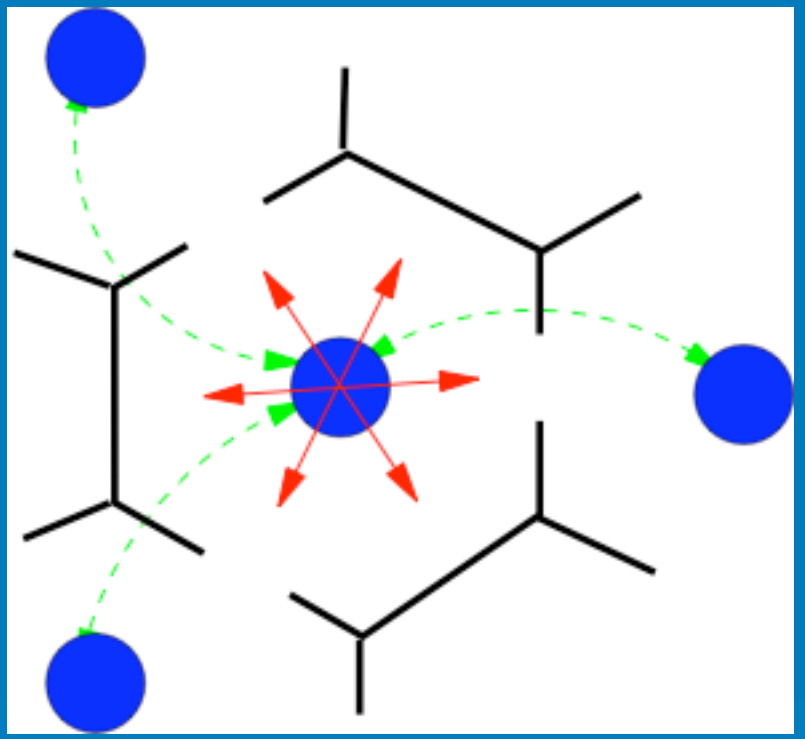
Na, K, Rb, Cs - symmetric mode



Stability of alkali site

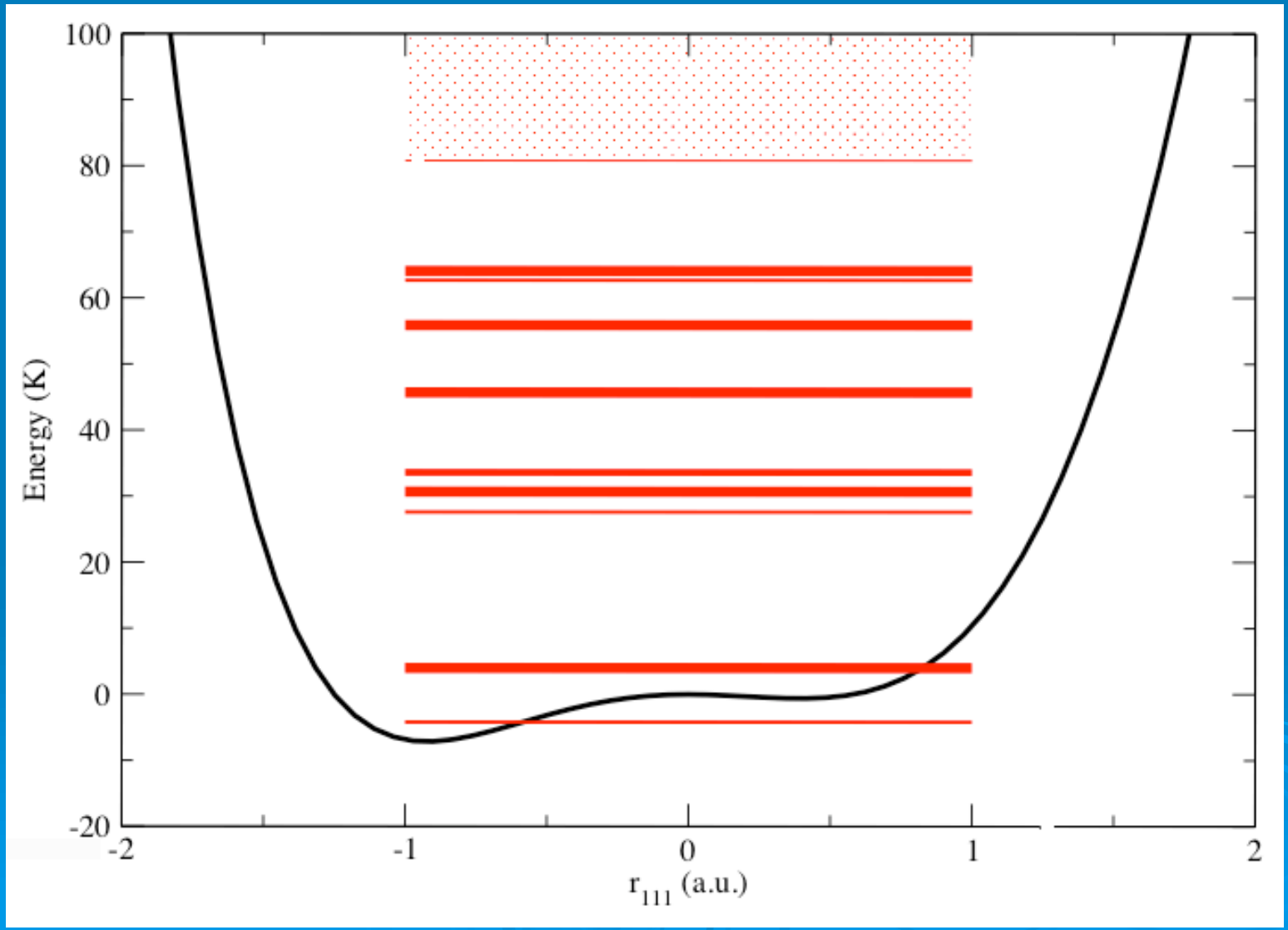
Site symmetry: l=0, 3, 4, 6,…

E(Δ) - polynomial fit (exp. ≥ 2)

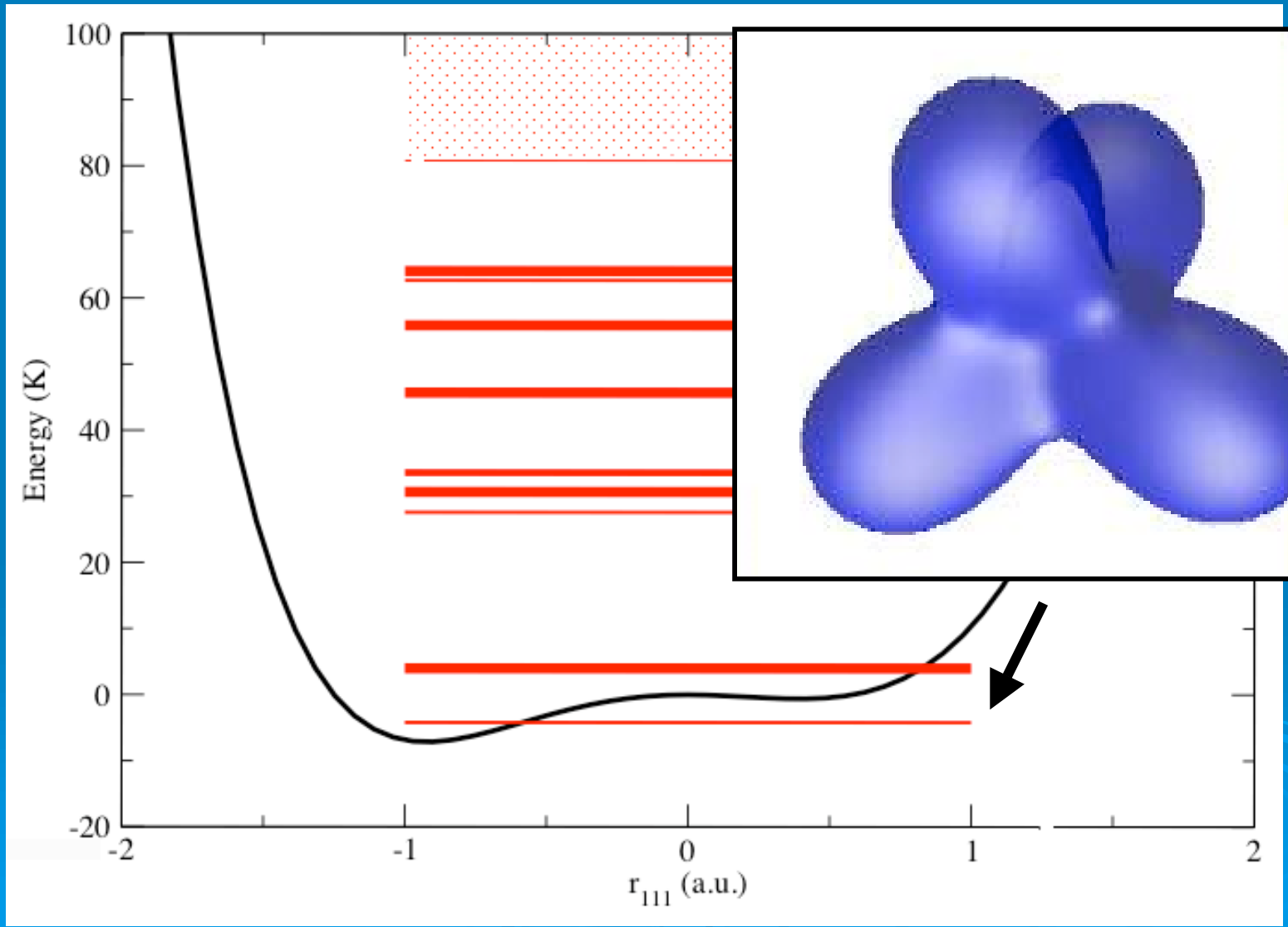


- On-site potential = Os-O cage + average K-K interaction
- K-K correlation

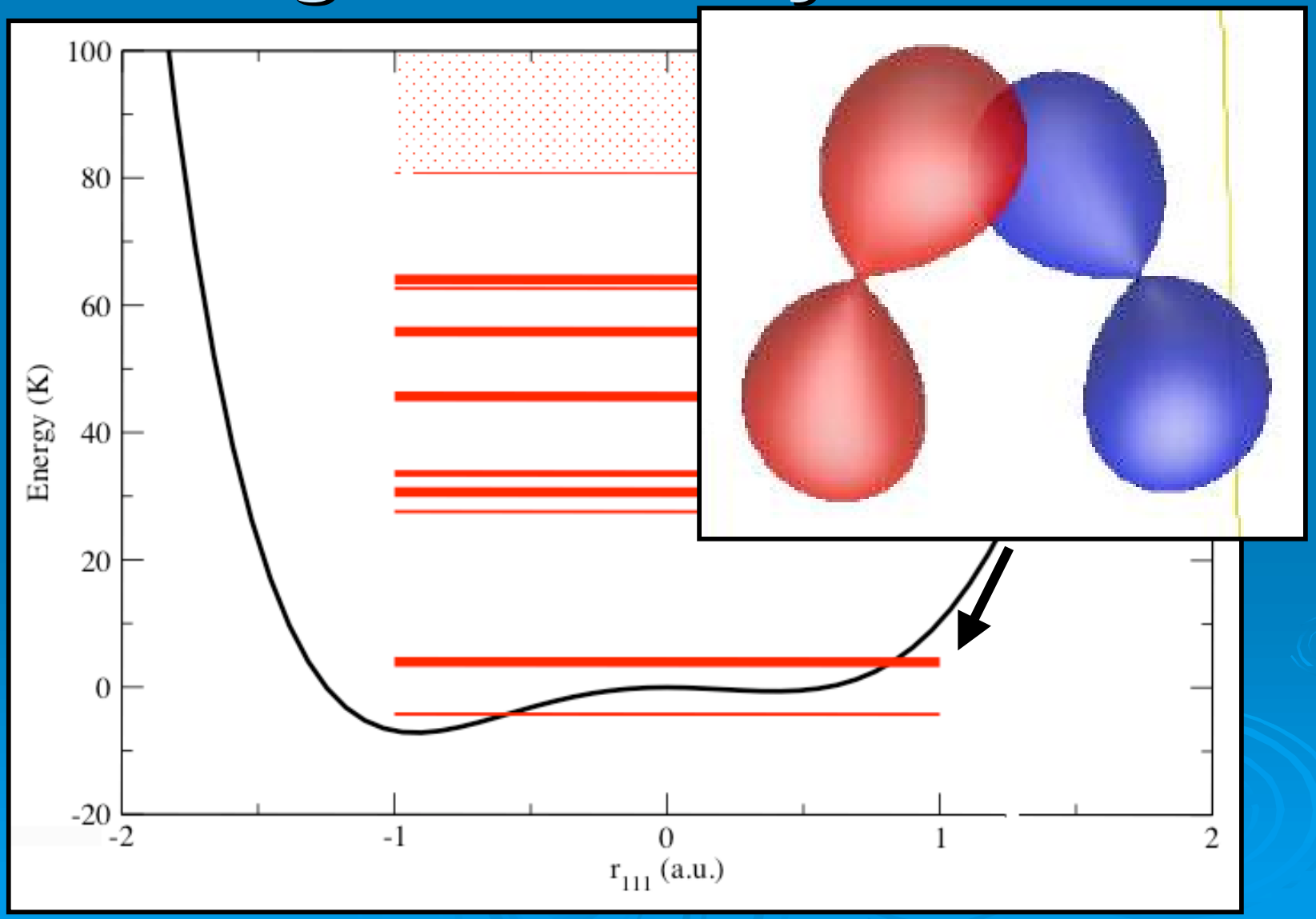
Single site K dynamics



Single site K dynamics



Single site K dynamics



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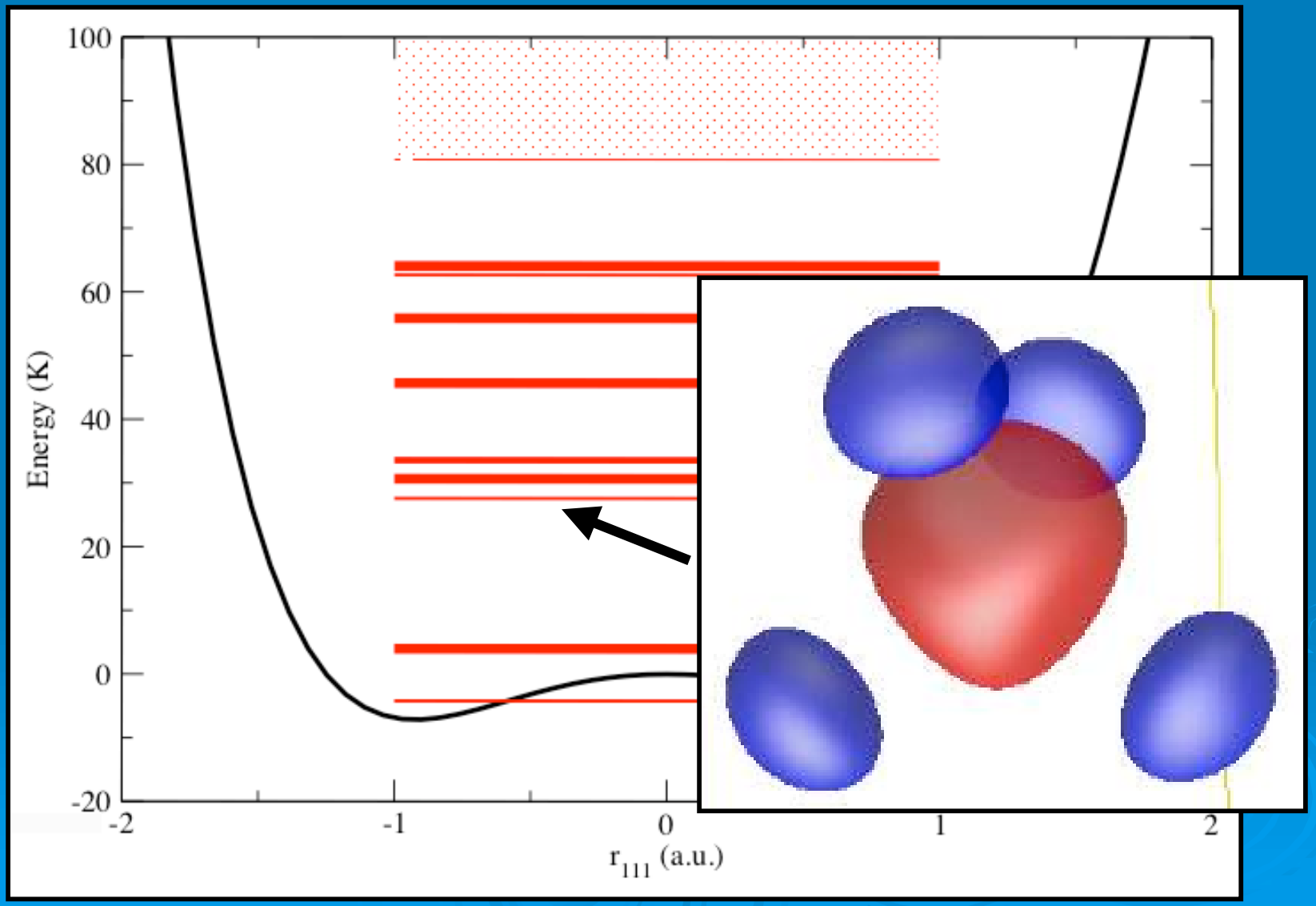

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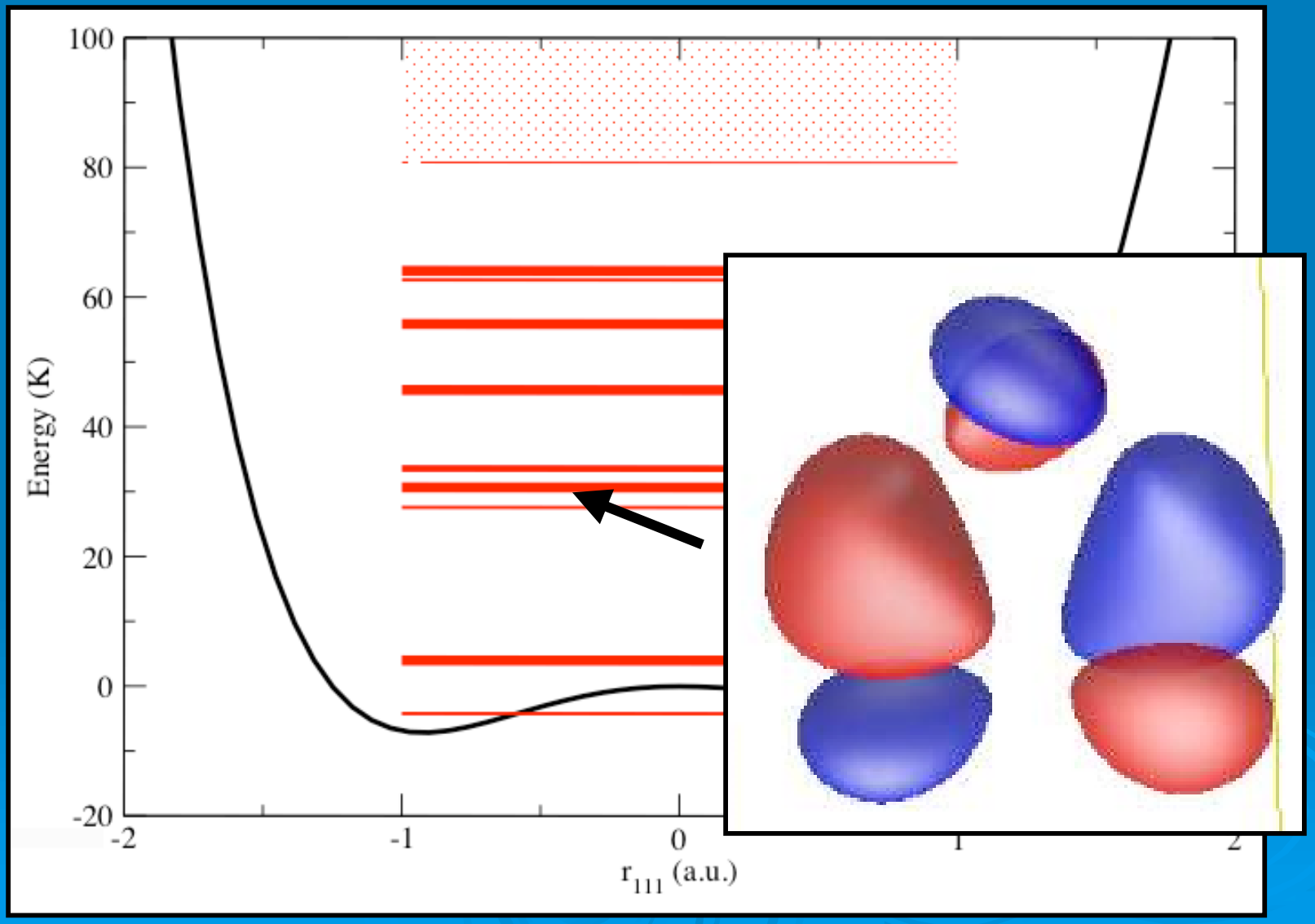
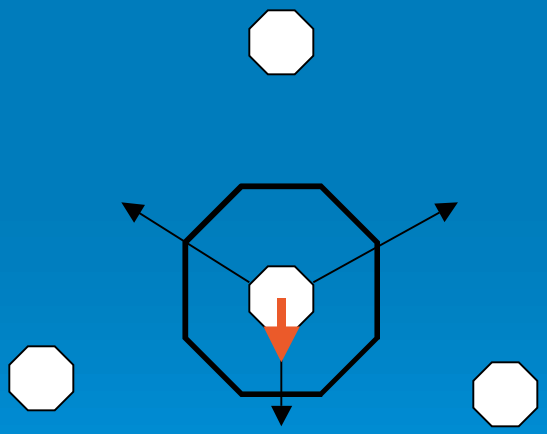
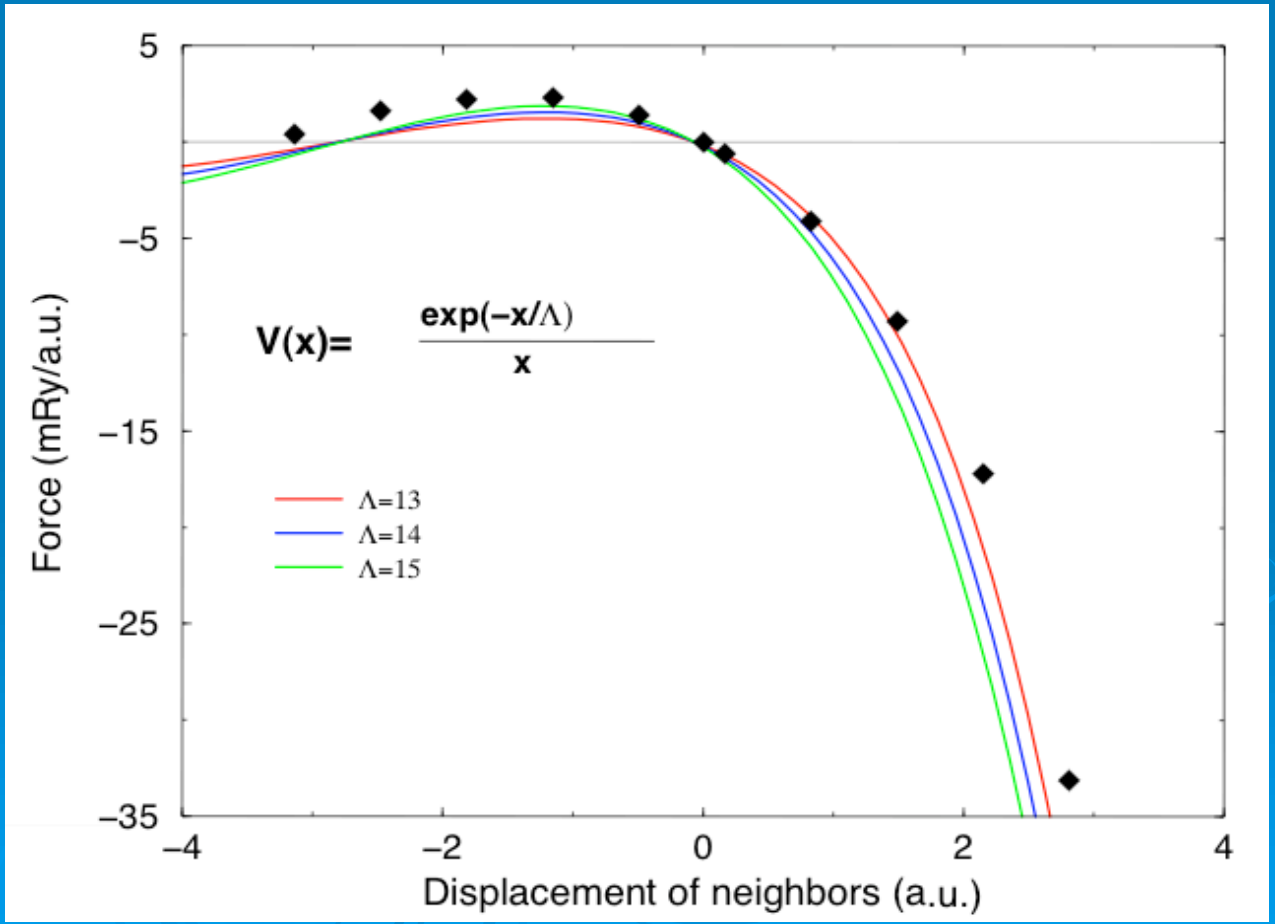


K-K interaction

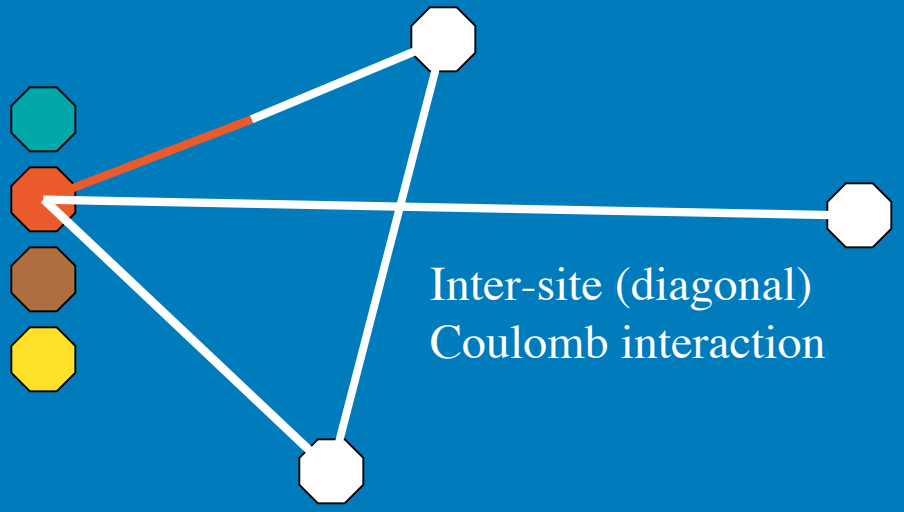
Calculated force acting of a static K ion, while its neighbors are displaced





Potts model

On-site (off-diagonal) terms



Inter-site (diagonal) Coulomb interaction

- No on-site term => anisotropic generalized Potts model q=4 on bipartite lattice (classical)
- On-site singlet-triplet splitting => off-diagonal terms (quantum)

Summary

- Dynamics of alkali ion is strongly size dependent
- K dynamics is anharmonic
- On-site ground state is a singlet-triplet split ($\Delta \sim 8$ K) => Schottky anomaly in specific heat
- K motion survives to low temperatures:
- NFL conductivity
- large D-W factor (anomalous T dependence)
- quadrupolar contribution to nuclear spin relaxation

*JK, T. Jeong, and W. E. Pickett Phys. Rev. B **70** 17510 (2004)*

Future outlook

Is there a phase transition in our model ?

What type ?

- Find classical ground state (degeneracy) => identify the order parameter.
- Mean field solution.
- Classical Monte-Carlo simulation.