'Electron-volt Neutron Spectroscopy: One Atom at a Time'
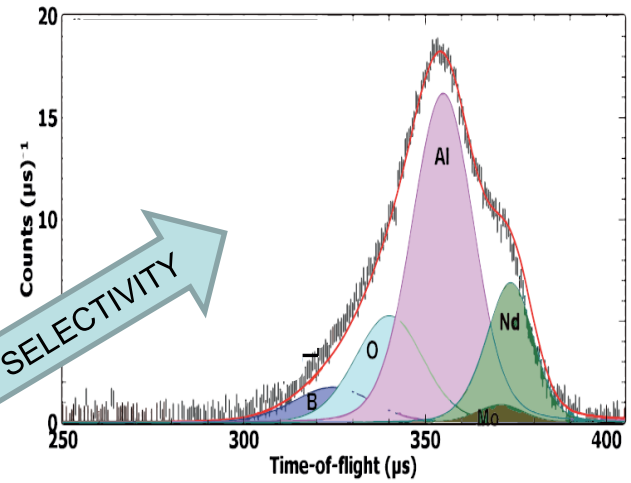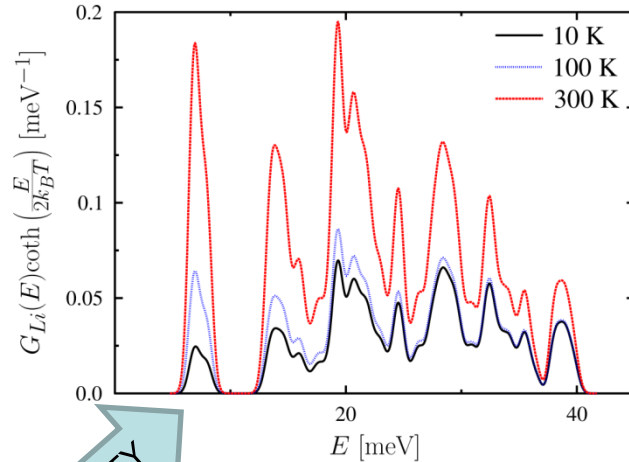<u>Matthew Krzystyniak</u>
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Mass-selective neutron Compton spectroscopy

No coupling constant weighting as PVDOS and cross section are separate parameters!

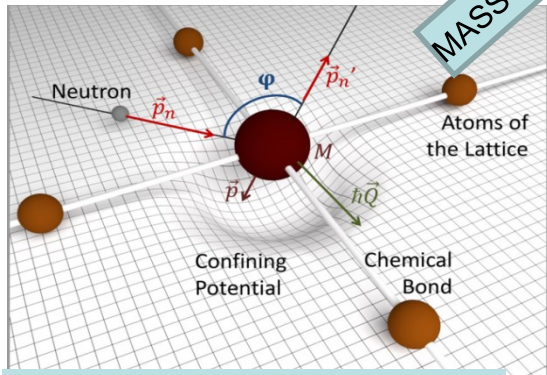**In many respects, an ultimate ab initio benchmarking tool!**

MASS SELECTIVITY

MASS SELECTIVITY

$$width\_M^2 \sim \int_0^\infty E \cdot G_M(E) \cdot coth\left[\frac{E}{2kT}\right] \cdot dE$$

first moment of the pVDOS!

$$partial\,VDOS = G_M(E) \cdot E \cdot coth\left[\frac{E}{2kT}\right]$$

PIMD

BOMD

LD from DFT

Ab initio modelling difficulty axis

$E \gg binding\ energy$

$Q \gg inverse\ interatomic\ distance$

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