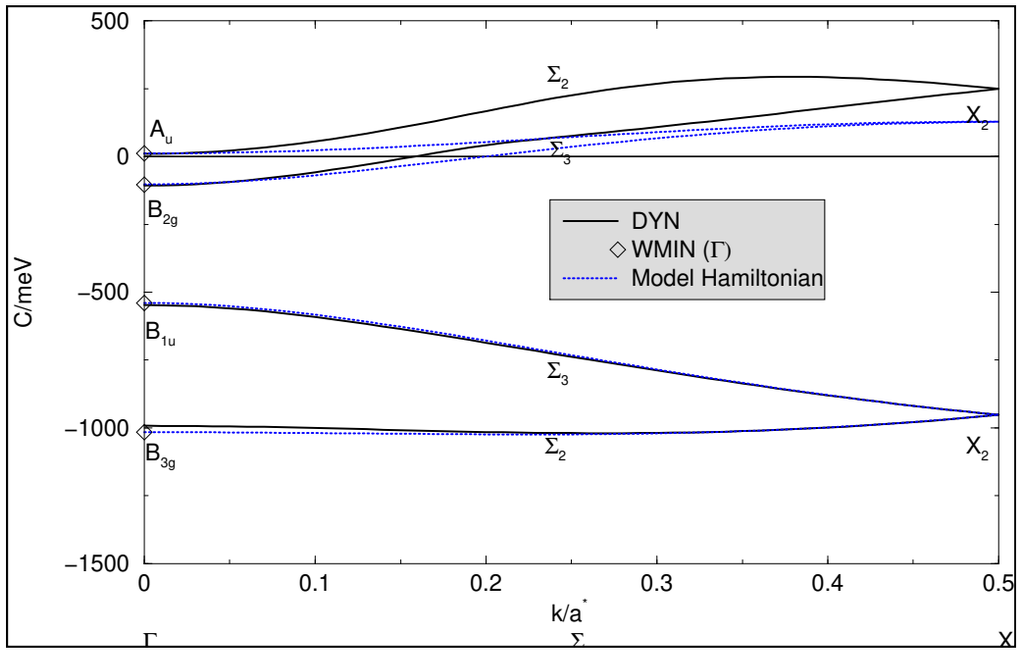
Comparison: Force constant model - Model Hamiltonian (couplings J)



Comparison: experimental - calculated elastic constants

$C_{k\ell}$	experiment	model
C_{11}	28.2 GPa	28.5 GPa
C_{22}	21.0 GPa	21.1 GPa
C_{33}	19.3 GPa	17.6 GPa
C_{44}		7.0 GPa
C_{55}		10.9 GPa
C_{66}	6.1 GPa	10.3 GPa
C_{12}	9.4 GPa	7.8 GPa
C_{13}	9.2 GPa	8.0 GPa
C_{23}	8.5 GPa	7.4 GPa