

**Table S1. Detailed Computational Parameters used in Quantum Espresso**

Parameter	Value / Setting	Description
<b>General &amp; DFT (Ground state)</b>		
<b>Codes</b>	pw.x, bands.x	Ground state density and bands
<b>Functional</b>	LDA (Perdew-Zunger)	Exchange-Correlation functional
<b>Pseudopotentials</b>	*.pz-vbc.UPF	Norm-conserving (VBC)
<b>Wavefunction Cutoff ( <math>E_{cut}^{wfc}</math> )</b>	120 Ry	Plane-wave basis cutoff
<b>Charge Density Cutoff ( <math>E_{cut}^{rho}</math> )</b>	480 Ry	Charge density basis cutoff
<b>k-point Sampling</b>	$3 \times 3 \times 3$	Monkhorst-Pack grid (DFT)
<b>Convergence Threshold</b>	$1.0 \times 10^{-6}$ Ry	SCF energy convergence criteria
<b>Mixing Scheme</b>	Thomas-Fermi (TF)	Charge density mixing mode
<b>Mixing Beta</b>	0.2	Mixing factor for SCF
<b>GW Calculations (gww.x)</b>		
<b>Module</b>	gww.x, head.x	GWW approximations
<b>Total Bands ( <math>N_{tot}</math> )</b>	525	Total Kohn-Sham states included
<b>Basis Size ( <math>N_{basis}</math> )</b>	97	Number of basis vectors (Principal Comp.)
<b>Fit Basis ( <math>N_{fit}</math> )</b>	120	Number of fit basis vectors
<b>Coulomb Cutoff</b>	True (l_truncated_coulomb)	Truncation for 2D slab geometry
<b>Frequency Grid</b>	5 (Gauss-Legendre)	Grid type on imaginary axis
<b>Time/Freq Points</b>	97	Number of points on imaginary axis
<b>Imaginary Time Range ( <math>\tau</math> )</b>	9.8 a.u.	Max imaginary time
<b>Energy Cutoff ( <math>\omega</math> )</b>	20.0 Ry	Basis energy cutoff
<b>Head Calculation</b>	Included (l_head=.true.)	Dielectric head ( $q \rightarrow 0$ ) treatment
<b>Phonon / Dielectric (ph.x)</b>		
<b>k-point Sampling</b>	$2 \times 2 \times 2$	Coarser grid for response calculation

<b>Convergence (<math>tr2\_ph</math>)</b>	$1.0 \times 10^{-7}$ Ry	Threshold for phonon/response
<b>Born Eff. Charges</b>	True (zeu)	Calculated for IR intensities
<b>Dielectric Matrix</b>	True (epsilon)	Calculated macroscopic dielectric const.
<b>Optical Properties (simple)</b>		
<b>Method</b>	IPA / GW-BSE	Independent Particle / BSE approx.
<b>Valence Bands (<math>N_v</math>)</b>	420	Number of valence bands in sum
<b>Conduction Bands (<math>N_c</math>)</b>	105	Number of conduction bands in sum
<b>Energy Range (<math>E_{max}</math>)</b>	1.1 Ry ( $\sim 15$ eV)	Max energy for optical spectrum
<b>Broadening</b>	0.0142 Ry ( $\sim 0.19$ eV)	Inter/Intra-band Lorentzian broadening
<b>Smearing Type</b>	Fermi-Dirac (-99)	Smearing method
<b>Smearing Width</b>	0.02205 Ry ( $\sim 0.3$ eV)	Electronic temperature for optics
<b>Interpolation</b>	True (4x4x4 grid)	Non-local commutator interpolation