

Table S1. Detailed Computational Parameters used in Quantum Espresso

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

Convergence (<i>tr2_ph</i>)	$1.0 \times 10^{-7} \text{ Ry}$	Threshold for phonon/response
Born Eff. Charges	True (zeu)	Calculated for IR intensities
Dielectric Matrix	True (epsil)	Calculated macroscopic dielectric const.
Optical Properties (simple)		
Method	IPA / GW-BSE	Independent Particle / BSE approx.
Valence Bands (N_v)	420	Number of valence bands in sum
Conduction Bands (N_c)	105	Number of conduction bands in sum
Energy Range (E_{max})	1.1 Ry (~ 15 eV)	Max energy for optical spectrum
Broadening	0.0142 Ry (~ 0.19 eV)	Inter/Intra-band Lorentzian broadening
Smearing Type	Fermi-Dirac (-99)	Smearing method
Smearing Width	0.02205 Ry (~ 0.3 eV)	Electronic temperature for optics
Interpolation	True (4x4x4 grid)	Non-local commutator interpolation
