Electronic supplementary information for

Large Excitonic Effect on van der Waals Interaction between Two-Dimensional Semiconductors

Jiabao Yang, Xiaofei Liu*, and Wanlin Guo

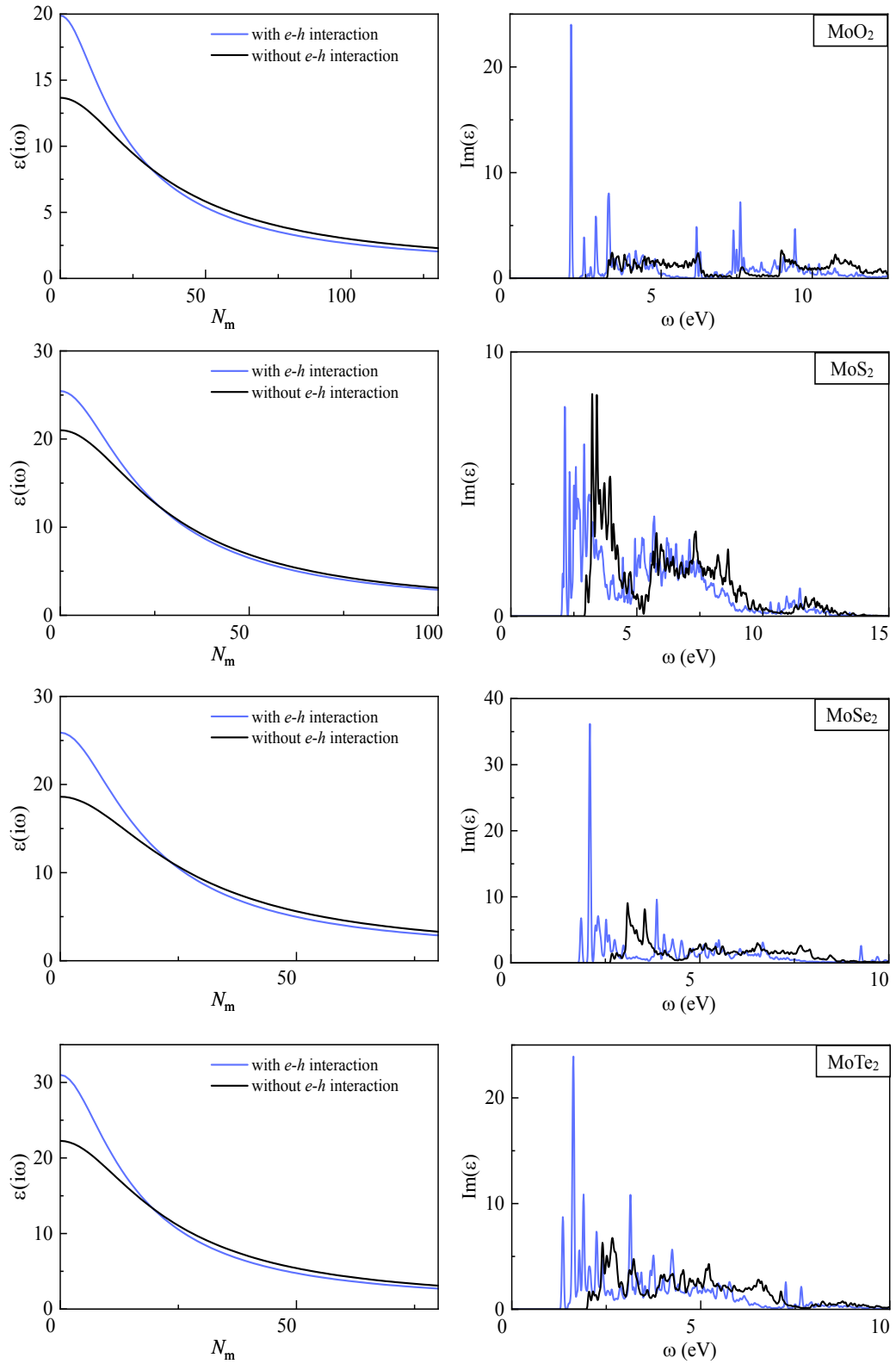
State Key Laboratory of Mechanics and Control of Mechanical Structures, Key Laboratory for Intelligent Nano Materials and Devices of Ministry of Education, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, China

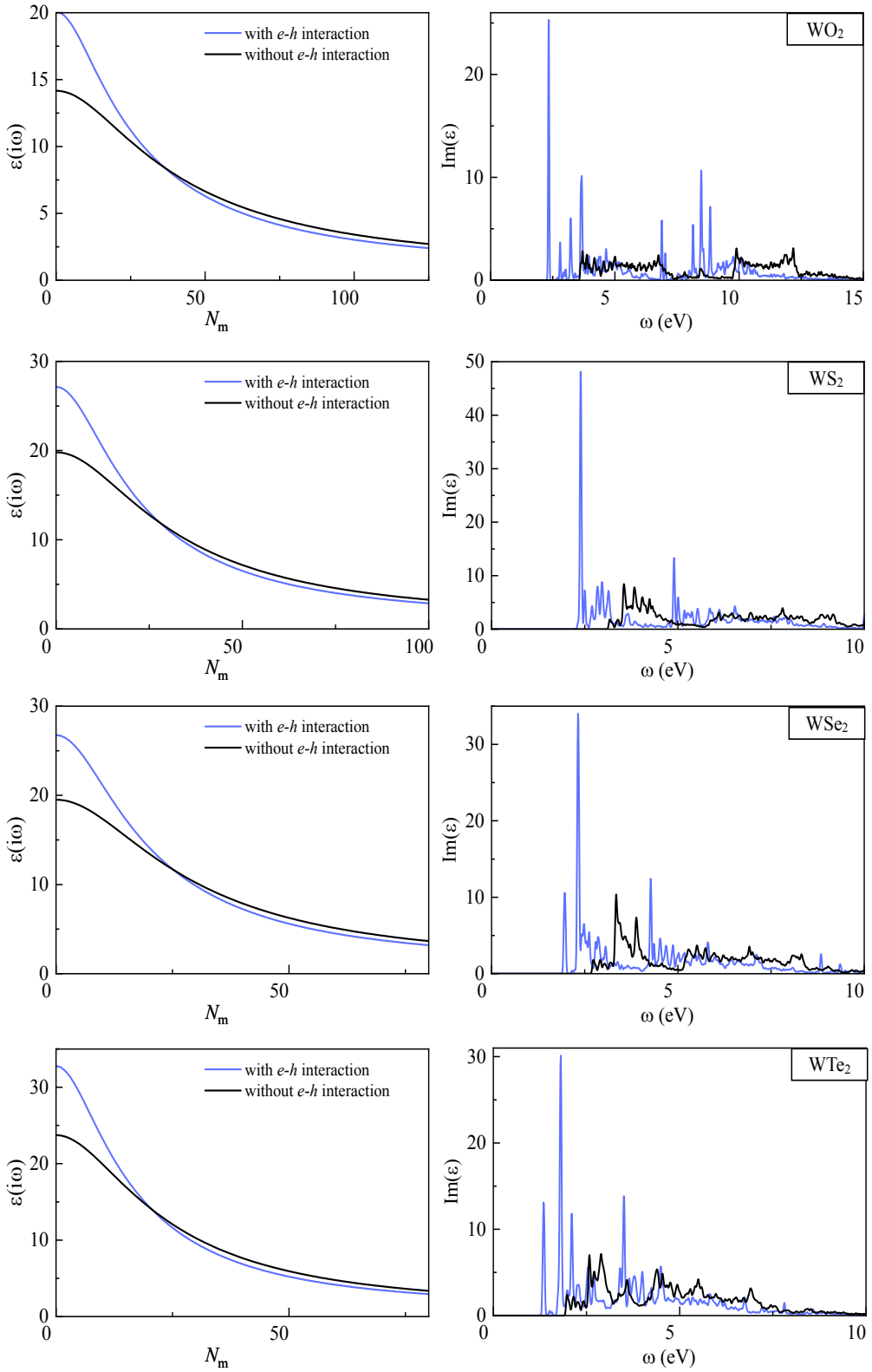
Table SI Lattice constants ***a***, effective thicknesses ***t***, the absorption edge energies with (E_{gap_eh}) and without the electron-hole (*e-h*) interaction (E_{gap_noeh}) of the representative two-dimensional semiconductors.

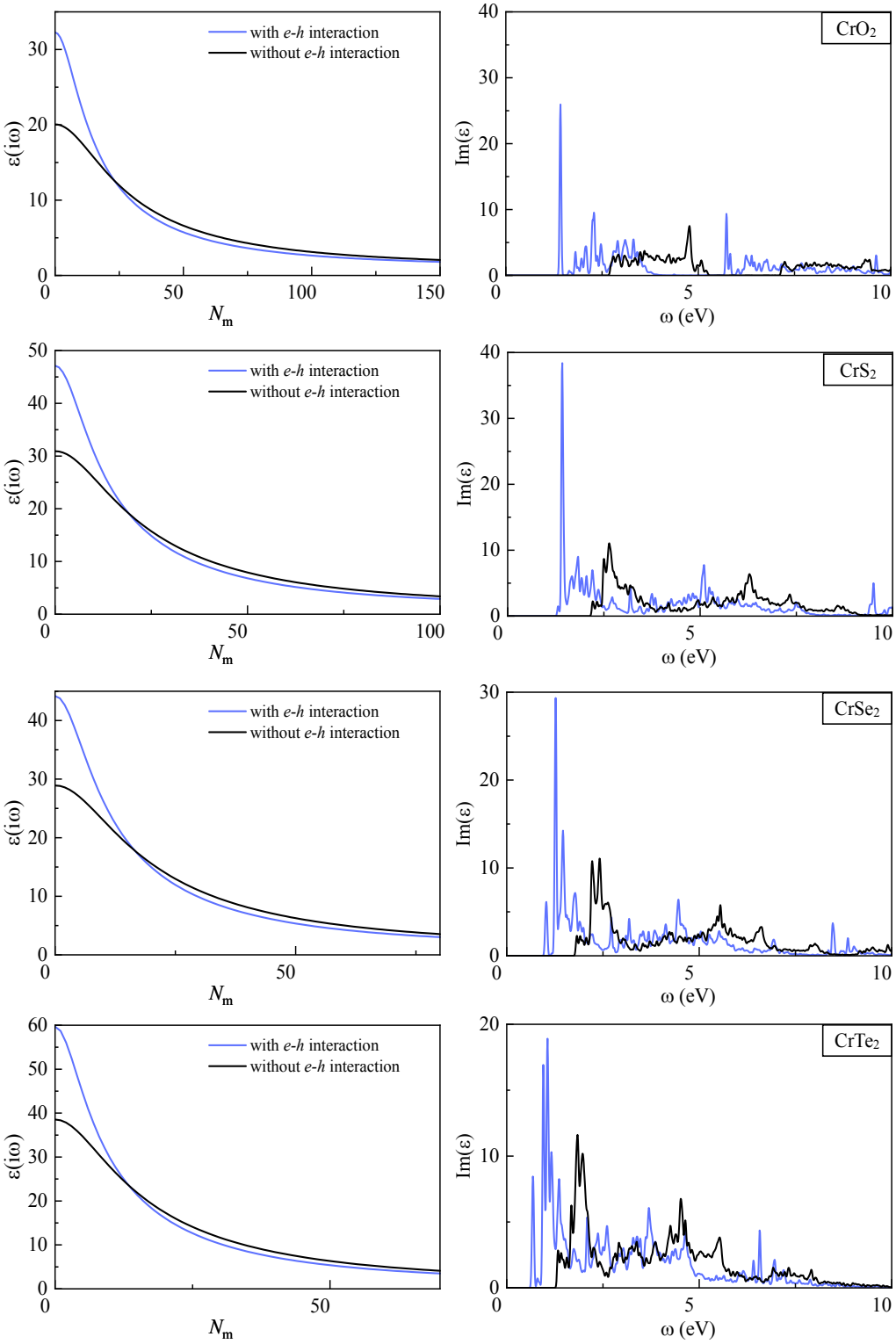
	a (Å)	***t*** (Å)	E_{gap_eh} (eV)	E_{gap_noeh} (eV)
BN	2.51	1.7	5.32	7.38
SiC	3.10	1.0	2.62	3.94
GeC	3.26	1.0	2.21	3.34
BNF	2.67	2.3	5.22	7.22
BNH	2.60	2.1	4.25	6.08
CF	2.61	2.3	5.01	6.99
CH	2.54	2.1	4.65	6.16
SiF	3.97	2.6	1.52	2.32
SiH	3.88	2.5	3.03	3.90
CrO_2	2.63	1.9	1.28	2.59
CrS_2	3.04	2.1	1.18	2.07
$CrSe_2$	3.21	2.3	0.88	1.68
$CrTe_2$	3.48	2.3	0.54	1.19
MoO_2	2.83	1.9	1.89	3.13
MoS_2	3.19	2.1	1.93	2.85
$MoSe_2$	3.32	2.3	1.72	2.54
$MoTe_2$	3.55	2.5	1.21	1.90
WO_2	2.84	1.9	2.20	3.41
WS_2	3.18	2.3	2.20	3.03
WSe_2	3.32	2.3	1.82	2.59
WTe_2	3.55	2.5	1.21	1.84
GaS	3.64	1.5	3.63	4.79
GaSe	3.82	2.0	3.01	3.73
SnO	3.84	1.4	3.31	4.72

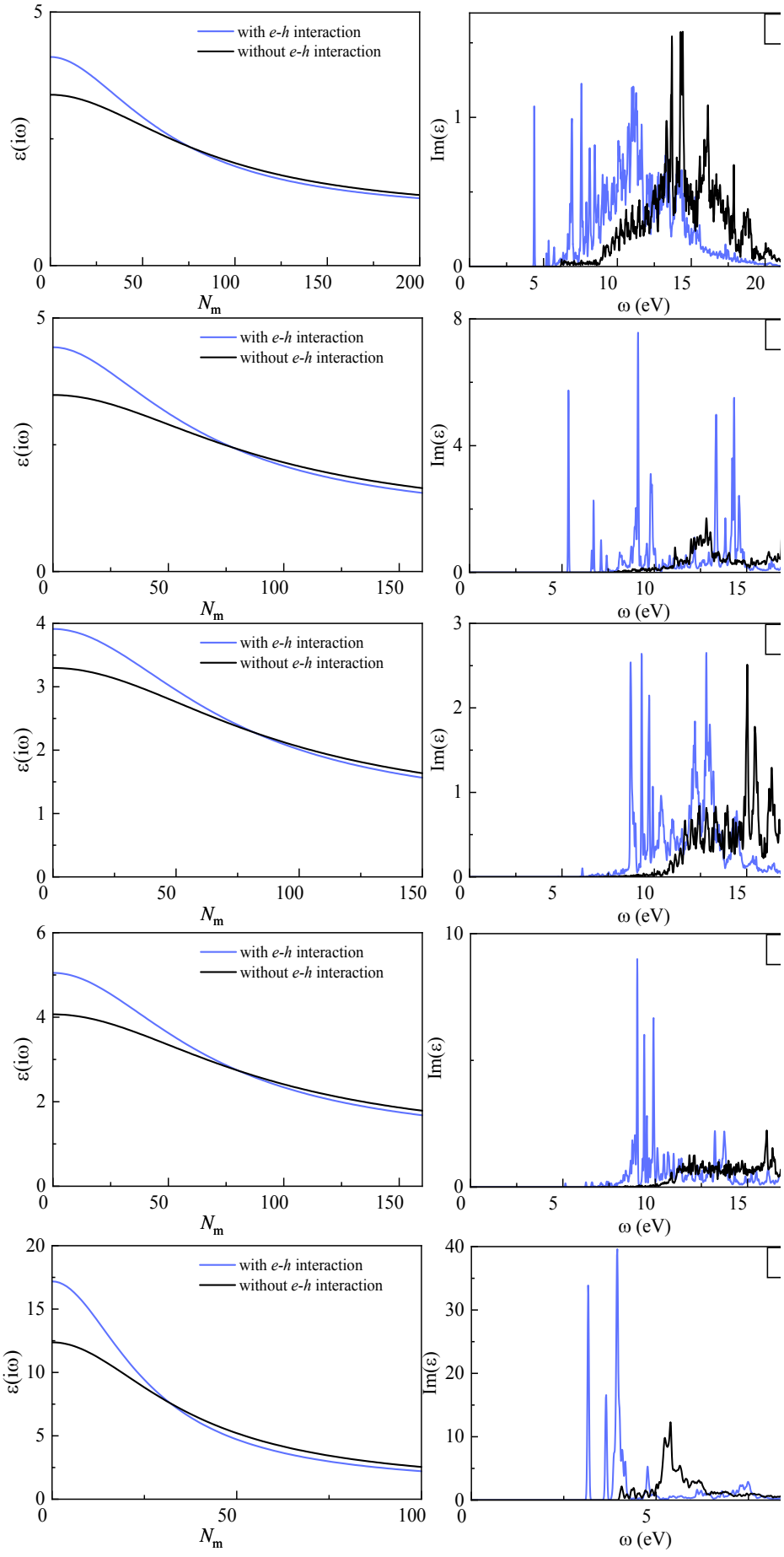
Table SII Critical frequencies ω_c at which the sign of E_{eh}-E_{noeh} changes from plus to minus, ratios of enhanced vdW energy by the *e-h* interaction at an interlayer distance of 10000Å and ratios of static dielectric constant with the *e-h* interaction to that without the *e-h* interaction for the semiconductors.

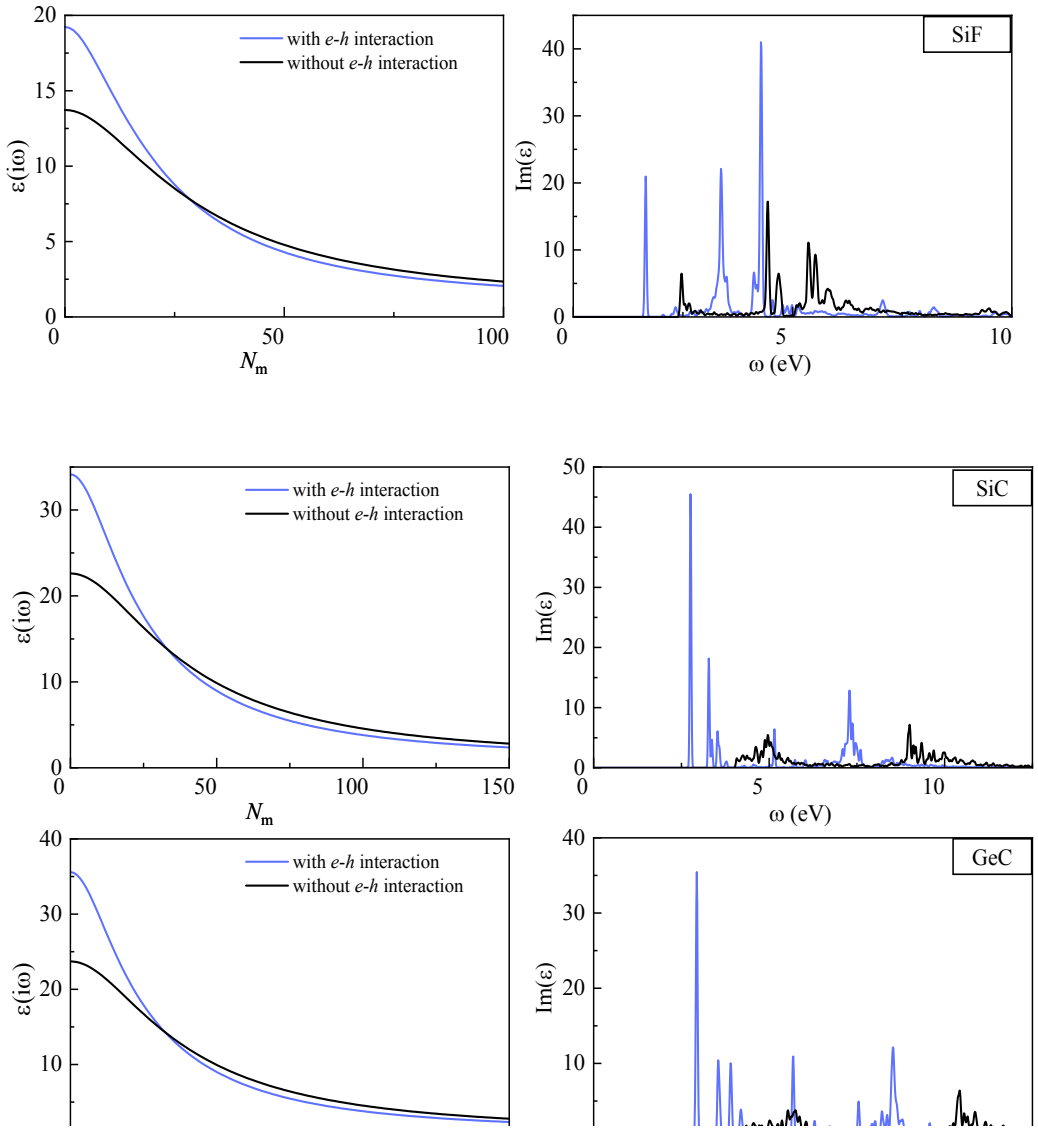
	ω_c (eV)	$(E_{eh}-E_{noeh})/E_{eh}$	$\varepsilon_{0\_eh}/\varepsilon_{0\_noeh}$
BN	7.95	0.24	1.39
SiC	4.93	0.29	1.50
GeC	5.41	0.30	1.51
BNF	12.24	0.22	1.27
BNH	11.92	0.18	1.22
CF	12.27	0.21	1.24
CH	12.88	0.17	1.19
SiF	4.45	0.25	1.40
SiH	4.93	0.26	1.39
CrO_2	3.66	0.31	1.61
CrS_2	3.02	0.29	1.52
$CrSe_2$	2.54	0.28	1.53
$CrTe_2$	2.07	0.28	1.55
MoO_2	4.93	0.26	1.46
MoS_2	4.13	0.15	1.21
$MoSe_2$	3.66	0.25	1.39
$MoTe_2$	3.02	0.24	1.39
WO_2	5.27	0.25	1.42
WS_2	4.29	0.24	1.37
WSe_2	3.80	0.25	1.37
WTe_2	3.18	0.24	1.38
GaS	6.04	0.24	1.31
GaSe	5.25	0.23	1.31
SnO	5.57	0.29	1.41


with e-h interaction
without e-h interaction
ε(iω)
N_m
Im(ε)
ω (eV)
MoO2
MoS2
MoSe2
MoTe2


with e-h interaction
without e-h interaction
ε(iω)
N_m
Im(ε)
ω (eV)
WO2
WS2
WSe2
WTe2


with e-h interaction
without e-h interaction
ε(iω)
N_m
Im(ε)
ω (eV)
CrO2
CrS2
CrSe2
CrTe2


with e-h interaction
without e-h interaction
ε(iω)
Im(ε)
N_m
ω (eV)


with e-h interaction
without e-h interaction
ε(iω)
N_m
Im(ε)
ω (eV)
SiF
SiC
GeC

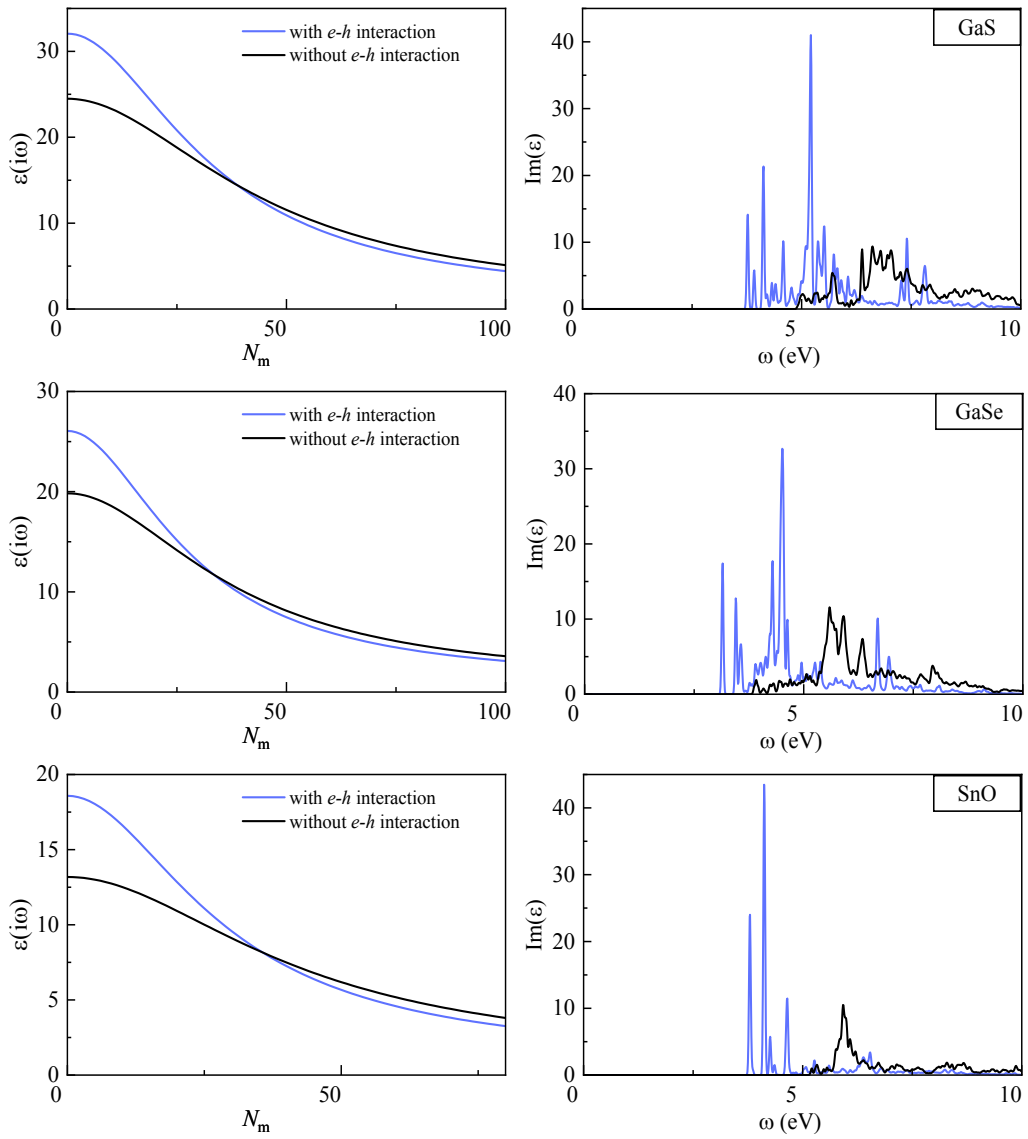


Fig. S1 Dielectric functions along the imaginary frequency axis and optical absorption spectra of all the considered two-dimensional semiconductors except for those shown in the main manuscript.

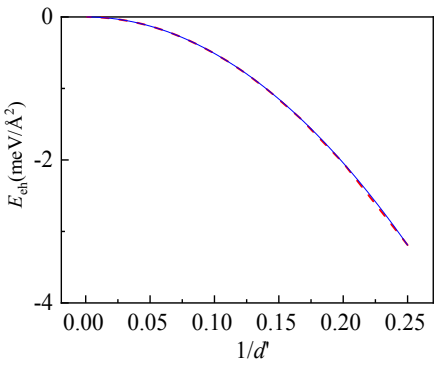


Fig. S2 VdW energies as a function of the inverse distance d' for semi-infinite surfaces of silicon. The E-1/d' relations in the distance range from 50 to 10000 Å are fitted by a power functions with an exponent of 2. The Chi-square tolerance for the fitting is set to 1×10^{-9}. The fitted results are visualized with the red dashed curves.

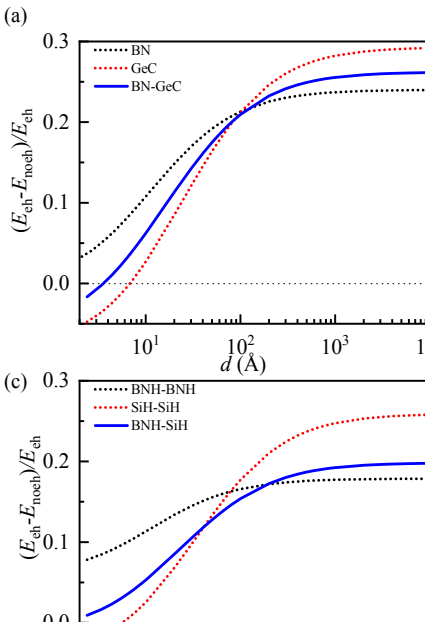


Fig. S3 Effect of the *e-h* interaction on the vdW energy as a function of distance for hetero-bilayers, including (a) BN-GeC, (b) CrO_2-CrS_2, (e) BNH-SiH, and (d) GaS-GaSe.