Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supplementary Information

Momentum and thickness dependent excitonic and plasmonic properties of 2D h-BN and MoS2 restored from supercell calculations

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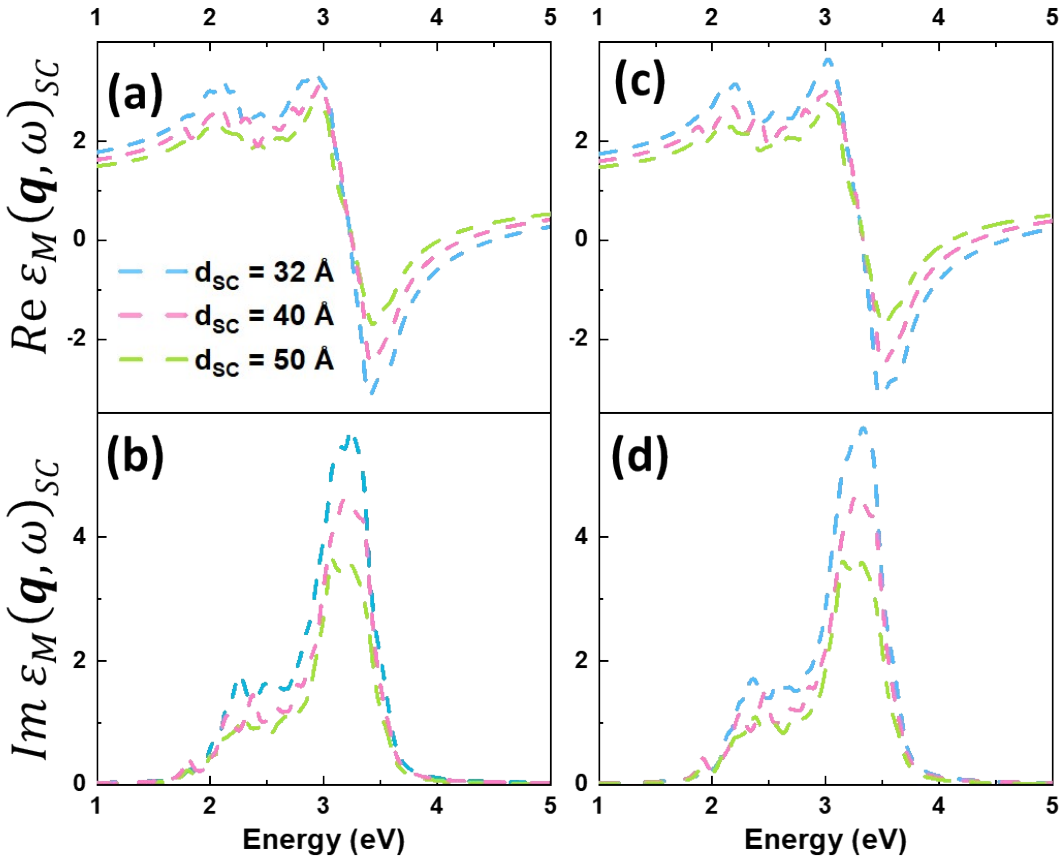

Fig. S1 Unrestored (a and c) real and (b and d) imaginary dielectric functions at finite momentum (|**q**| = 0.05 Å^{-1}) along ΓM of monolayer MoS_2 calculated within the many body perturbation theory with different vacuum volumes, resulting different supercells thicknesses d_{SC} from 32 Å, 40 Å to 50 Å. Note that the dielectric functions in (a-b) are calculated with the Coulomb truncation while the dielectric functions in (c-d) are calculated without the Coulomb truncation.

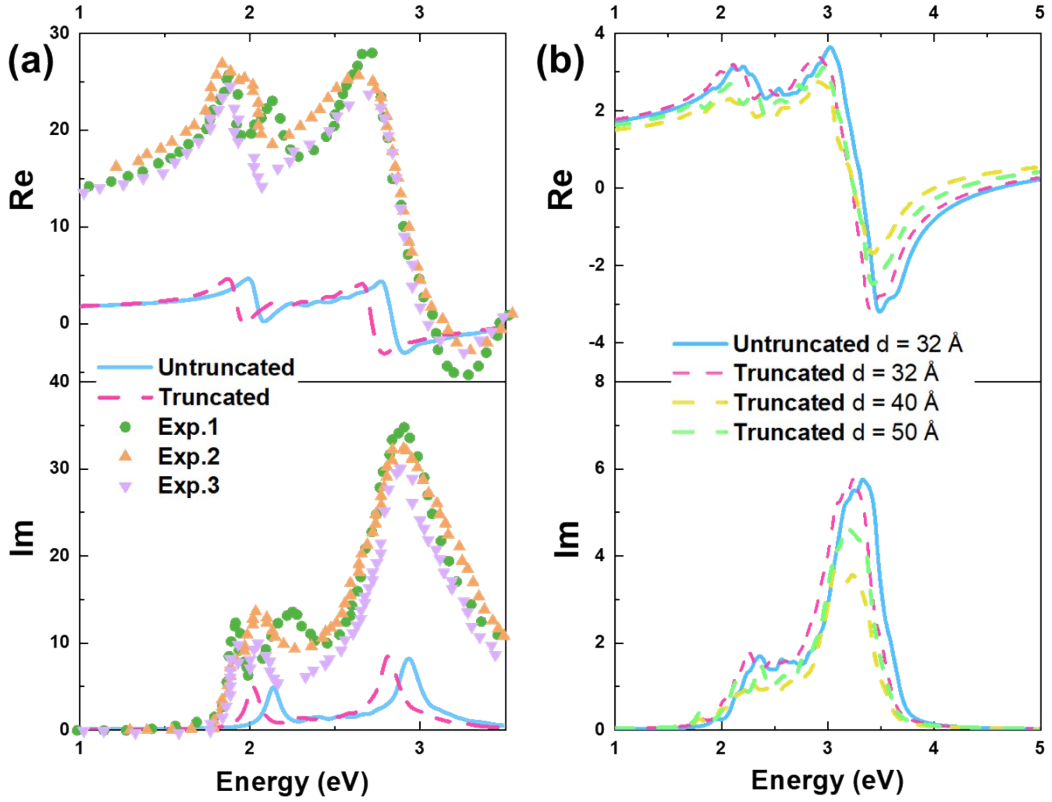

Fig. S2 The dielectric functions of monolayer MoS_2 at (a) **q** = 0 and (b) **q** = 0.05 $Å^{-1}$. Note that the untruncated and truncated results are depicted in full lines and dashed lines, respectively, compared with experimental results [1-3] in dots. The thicknesses of supercells are also noted in (b).

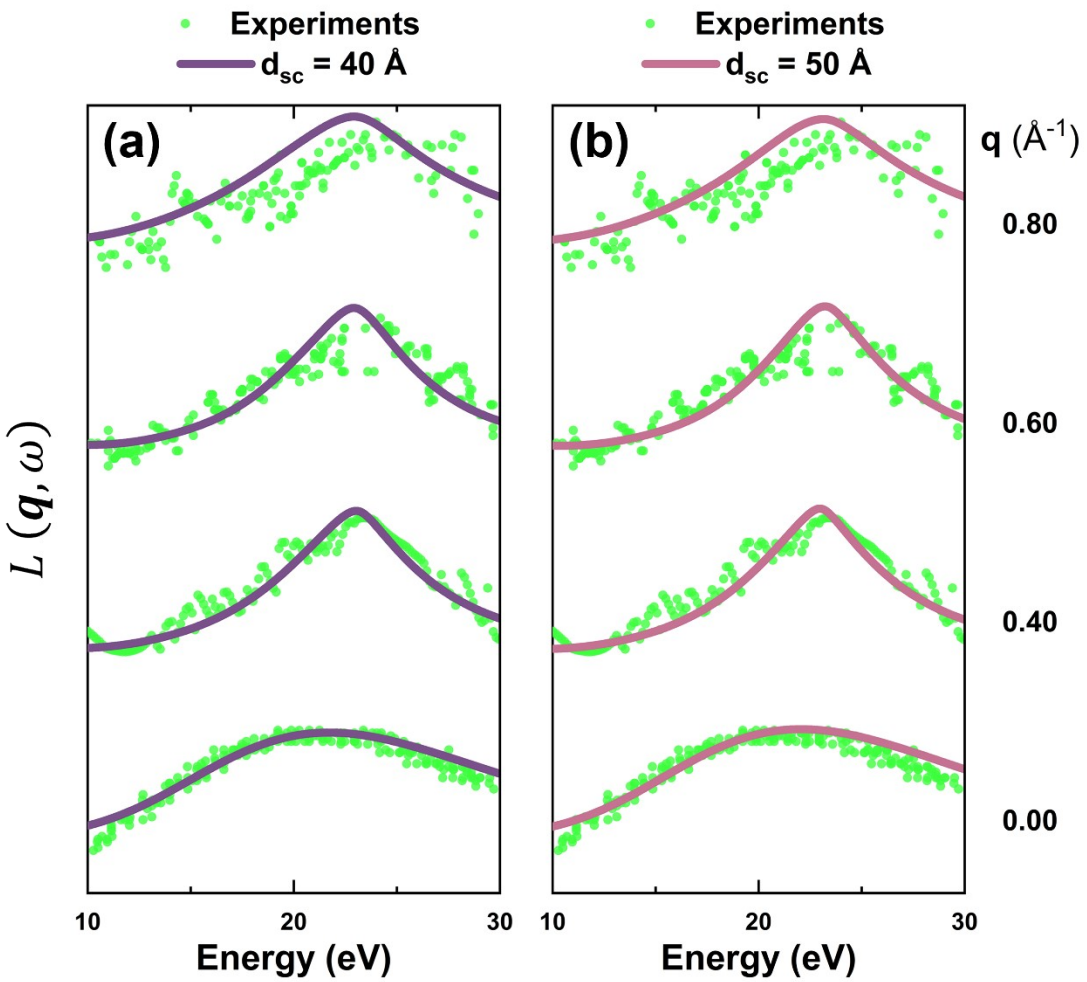

Fig. S3 The restored energy-loss functions of monolayer MoS_2 compared with experimental measurements [4, 5] (green dots) from vanishing **q** to finite **q** along ΓM. The restorations are based on different supercell thicknesses of (a) 40 Å and (b) 50 Å.

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