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Supplementary Material for

"Wurtzite MgSe: a promising candidate with the excellent visual light transparence and p-type conductivity"

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I. Cutoff energy

The cut-off energy for plane-wave is set up as 250.0 eV. The energies of host atoms Mg and Se are both below 250.0 eV, whereas the cutoff energy of impurity atom N notably exceeds this value. Hence, the convergence testing of the cutoff energy is carried out, and the results are depicted in Fig. S1. The results indicate that the cutoff energy is set to 420.0 eV, the energy difference is less than 0.1 eV, meeting the convergence criterion. Therefore, the cutoff energy with respect to N are all set to 420.0 eV.

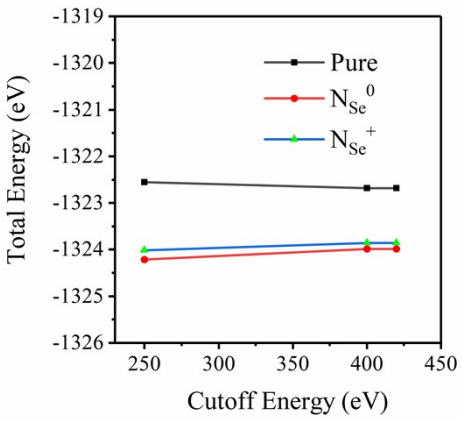

Fig. S1. (Color online) The total energies of defect N_{Se}, varying with cutoff energies, are shown.

II. Electronic Structure

We employed the HSE06 scheme to compute the band structure of RS, ZB and NiAs structures, with the results presented in Fig. S2. The findings reveal that RS exhibits a bandgap of 2.61 eV, consistent with Liu *et al.*'s calculations.[1] The ZB structure displays a direct bandgap of 3.52 eV. Similarly, the NiAs structure shows a

bandgap of 3.25 eV, as depicted in Fig. S2(c).

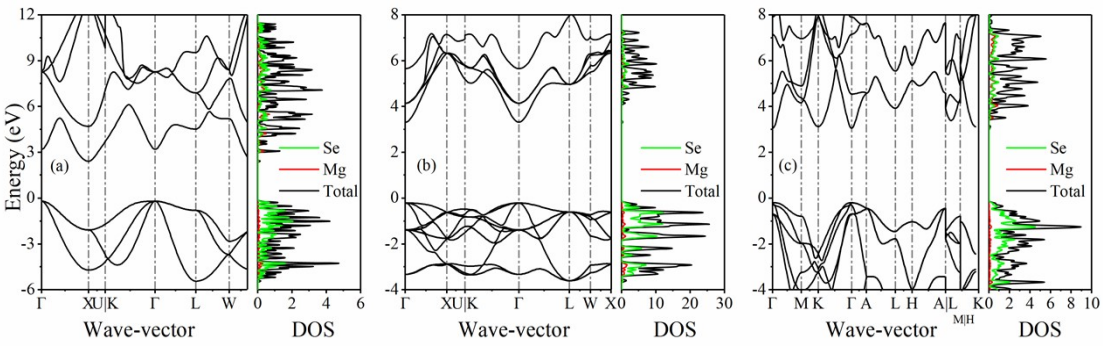

Fig. S2. The electronic structure of (a) rock-salt, (b) zinc-blende, and (c) NiAs MgSe are calculated by HSE06. The right panel is the density of states for the total and each host atoms.

III. Optical properties

We compute the transmittance of the rock-salt (RS), zinc-blende (ZB), and NiAs phases and plot in Fig. S3. It is shown that the RS and ZB phases are cubic crystal structures and the lattice constants are the same in all three directions, exhibiting isotropy. However, the transmittance of the RS structure is lower than that of the ZB structure in the visible light range. As the thickness of the sample increases, the transmittance of the RS structure in the UV range decreases dramatically. In contrast, when the sample thickness is 100 nm, the transmittance of the ZB structure to visible light is still as high as 80%. The NiAs phase is a hexagonal crystal like the wurtzite phase and exhibits anisotropy in the *x*(*y*) and *z* directions. Smaller differences exist in *x*(*y*) and *z* directions. When the thickness of the sample is increased to 100 nm, 70% transmittance is achieved in both directions.

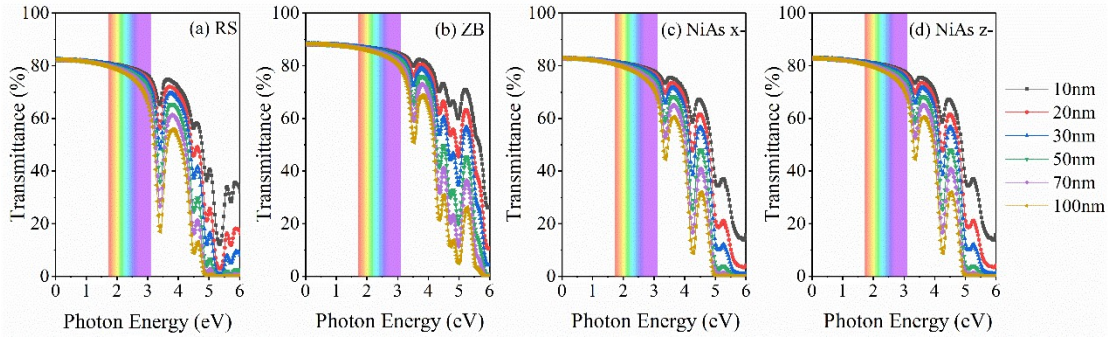

Fig. S3. The transmittance of (a) rock-salt, (b) zinc-blende, (c) NiAs *x*-direction, and (d) NiAs *z*-direction are calculated by HSE06.

IV. Hole effective mass

Table 1. The calculated hole effective mass in rock-salt and zinc-blende structures, along the different directions, are shown.

	Γ-X	Γ-K	Γ-L
RS	0.754	17.374	2.078
ZB	11.229	3.130	2.865

Table 2. The calculated hole effective mass in NiAs structure, along the different directions, are shown.

	Γ-K	Γ-A
NiAs	0.316	2.686

V. The distance of Se-Mg

The distance (Å) between the dopant with their nearest neighboring Mg atom, before and after optimization, are listed.

Optimization		
	Se-Mg	N-Mg
Distance	2.59	2.05

VI. The calculated of Fermi energy, defect concentration, and free carrier density

Based on the Eq. (2)-(8), we simulate the hole density for N-doped MgSe from different growth temperature quenched to room temperature. And the corresponding results are present in Fig. S4.

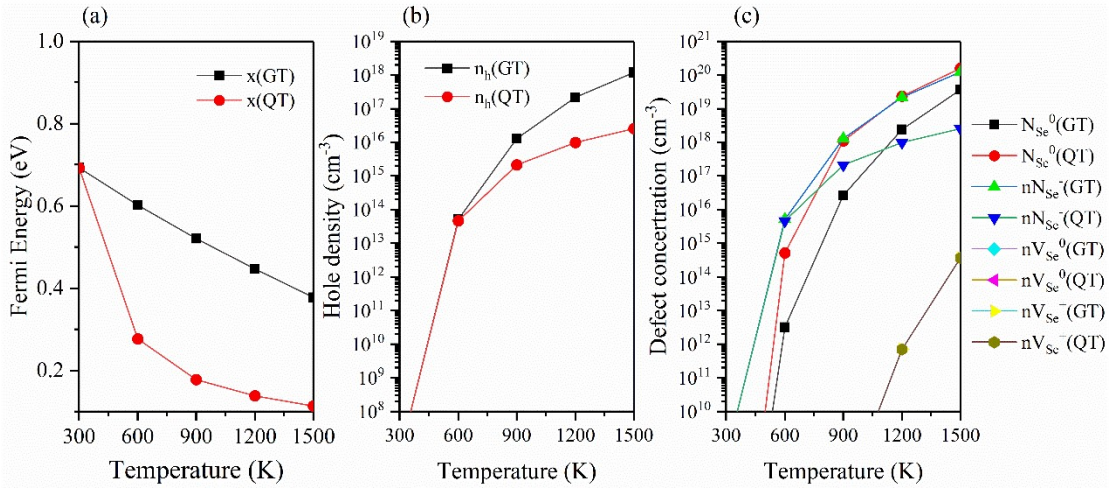

Fig. S4. The Fermi energy, hole density, and ionized defect concentrations in N-doped MgSe are plotted (a)-(c). GT(RT) represents the results calculated at growth temperature (after rapid quenching to room temperature).

References

1 M. Zhong, W. Zeng, F. Liu, D. Fan, B. Tang and Q. J. Liu, *Materials Today Physics*, 2022, **22**, 100583.