Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary information

Finite-momentum excitons and role of electron-phonon couplings to electronic and phonon transport properties in boron arsenide

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Table S1. Calculated high frequency dielectric constants ϵ_∞, static dielectric constants ϵ_0, averaged longitudinal elastic constant C and POP frequencies ω_{POP} for strain-engineering BAs.

strain type	**strain(%)**	ϵ_∞	ϵ_0	C **(GPa)**	ω_{POP} **(THz)**	m_e (m_0)	m_h (m_0)
unstrain	0	10.14	10.28	262.41	20.24	0.252	0.237
uniaxial	-4	10.13	10.42	296.41	20.27	0.254	0.186
	-3	10.07	10.35	288.04	20.32	0.257	0.201
	-2	10.28	10.17	279.48	20.82	0.257	0.217
	-1	10.16	10.2	271.11	21.27	0.259	0.237
	1	10.23	10.29	255.36	21.54	0.275	0.237
	2	10.13	10.33	248.68	21.63	0.278	0.221
	3	10.25	10.31	242.01	21.39	0.277	0.214
	4	10.25	10.3	235.44	21.84	0.276	0.216
	5	10.24	10.28	229.12	22.04	0.277	0.224
	6	10.22	10.26	223.05	22.18	0.274	0.233
triaxial	-4	12.64	12.87	335.28	22.09	0.154	0.186
	-3	12.44	12.77	323.59	22.15	0.157	0.201
	-2	12.4	12.51	305.58	21.89	0.157	0.217
	-1	11.7	11.77	285.15	20.23	0.159	0.237
	1	10.65	10.77	251.45	20.26	0.275	0.237
	2	10.46	10.65	245.18	20.86	0.278	0.221
	3	10.49	10.57	241.59	21.28	0.277	0.214
	4	10.65	10.68	236.41	22.32	0.276	0.216
	5	10.68	10.71	228.31	22.43	0.277	0.224
	6	10.79	10.81	222.61	22.92	0.274	0.233

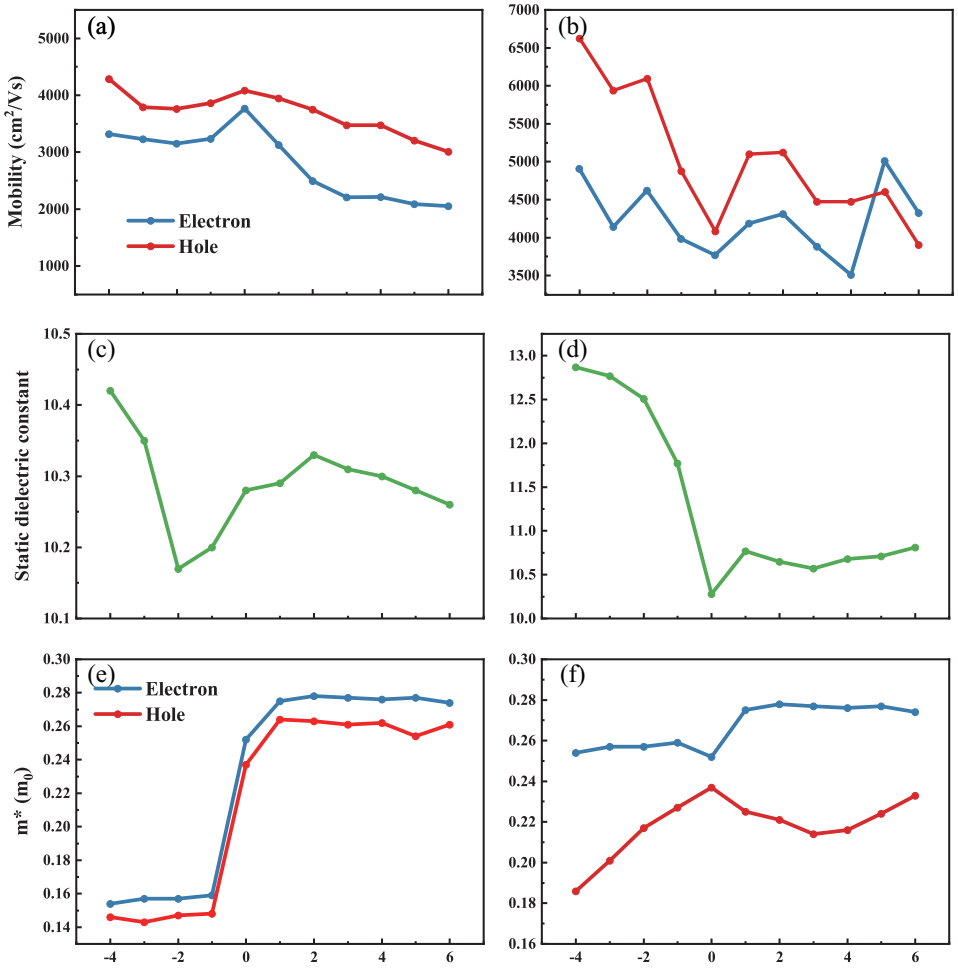

Figure S1. Mobility under different strains along (a) uniaxial directions, (b) triaxial directions. Static dielectric constant of BAs under different strains along (c) uniaxial directions, (d) triaxial directions. Effective mass under different strains along (e) uniaxial directions, (f) triaxial directions.

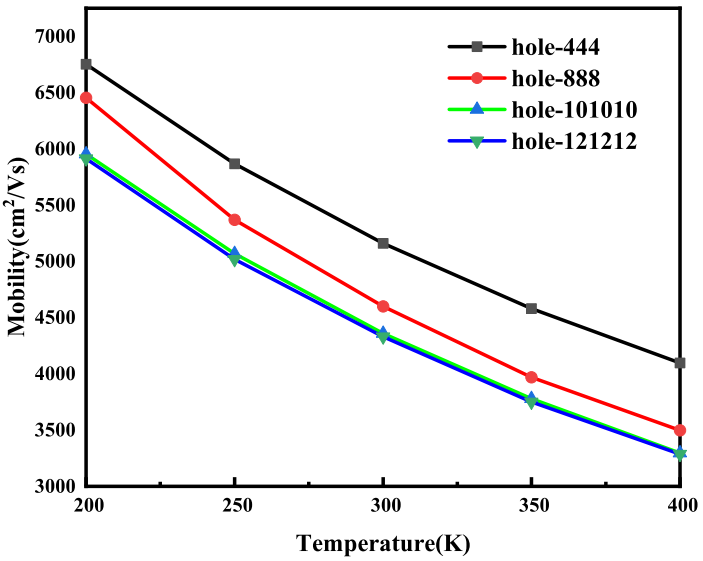

Figure S2. The convergence test of dense mesh which was used to compute scattering rates in AMSET.

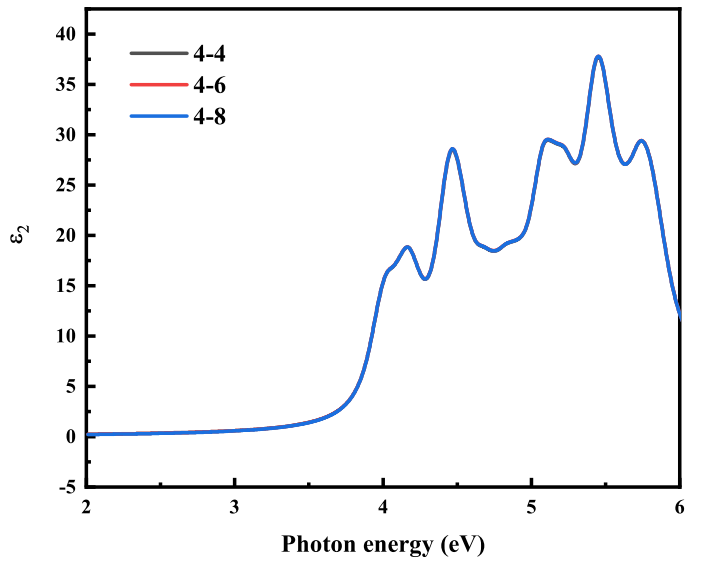

Figure S3. The convergence test for the BSE calculations by choosing the numbers of valence and conduction bands as (4,4), (4,6) and (4,8), and the calculated energy-dependent imaginary part of the dielectric functions.