Supporting information

The morphology-dependent lattice stability investigation in ZnS nanostructures by high-pressure XAFS studies

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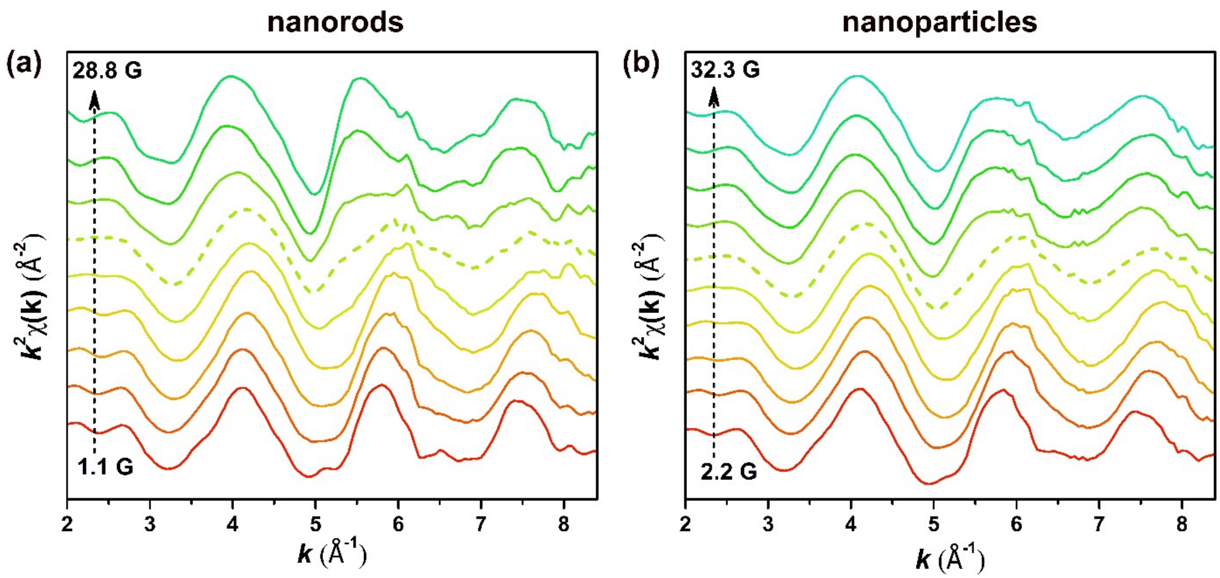

Figure S1. Extracted k^2-weighted XAFS spectra, $k^2\chi(k)$, for ZnS (c) nanorods and (d) nanoparticles at elevated pressures. The spectra in dashed lines represent the start of transition. The spectra are vertically shifted.

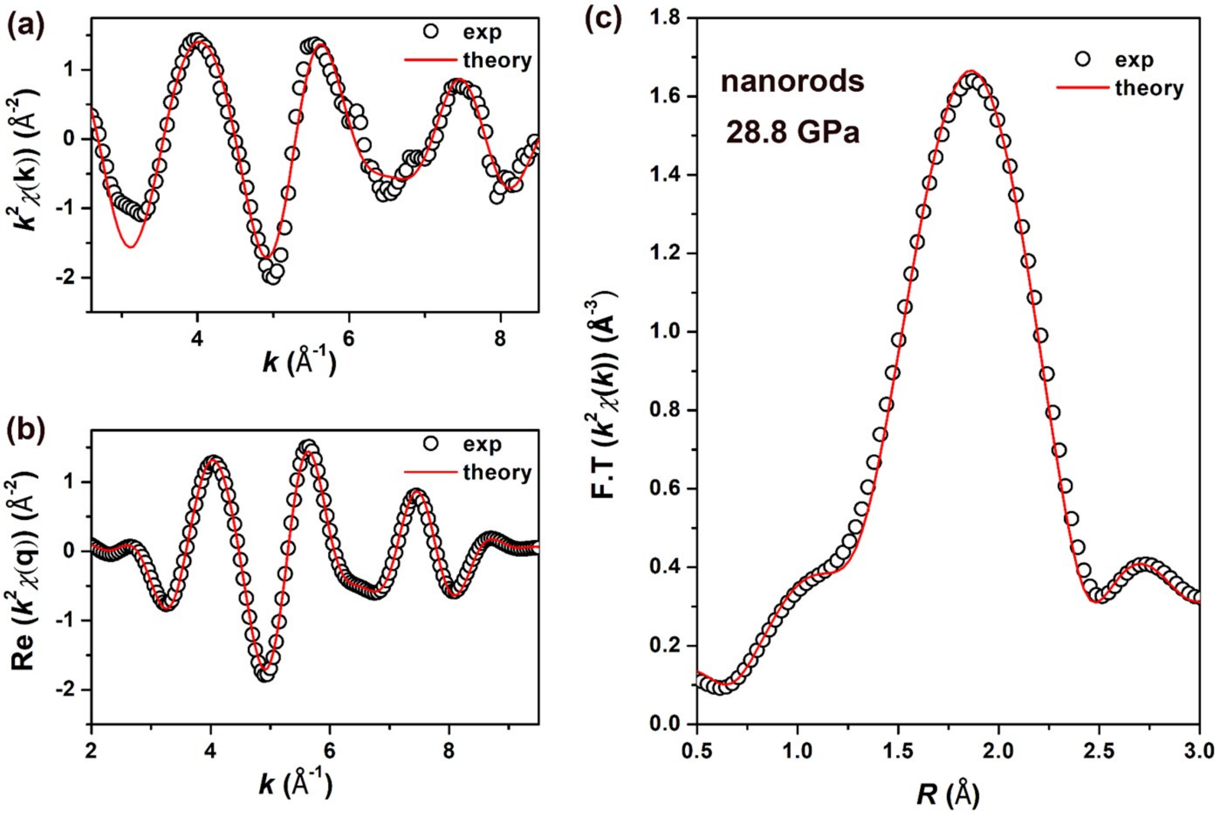

Figure S2. Comparison between the experimental EXAFS spectra and the best-fits corresponding to a single-distance shell at 28.8 GPa for ZnS nanorods. (a) and (b) show the extracted $k^2\chi(k)$ signal the back-transformed $k^2\chi(q)$ signal. (c) is the comparison in the R space.

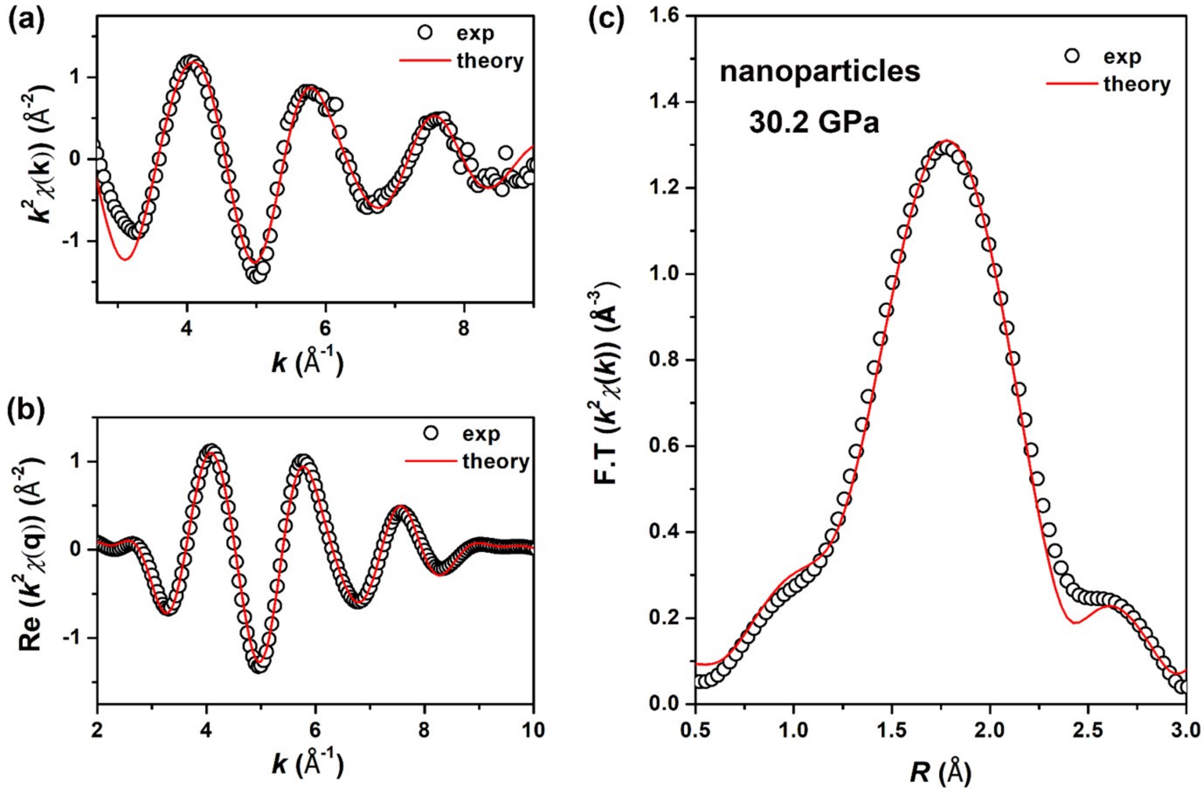

Figure S3. Comparison between the experimental EXAFS spectra and the best-fits corresponding to a single-distance shell at 30.2 GPa for ZnS nanoparticles. (a) and (b) show the extracted $k^2\chi(k)$ signal the back-transformed $k^2\chi(q)$ signal. (c) is the comparison in the *R* space.

Table S1. Fitting results of the first shell Zn-S distance, σ^2, S_0^2, ΔE_0, and *R*-factor at selected pressures for ZnS nanorods.

P (GPa)	*N*	*Zn-S distance (Å)*	*σ^2 (Å^2)*	S_0^2	*ΔE_0 (eV)*	*R-factor*
0	4	2.337±0.008	0.0066±0.0011	1.00	3.459	0.0068
1.1	4	2.336±0.012	0.0054±0.0014	0.91	4.426	0.0095
3.3	4	2.325±0.015	0.0069±0.0023	1.05	4.309	0.0108
5.3	4	2.317±0.016	0.0077±0.0026	1.08	3.303	0.0168
9.5	4	2.300±0.012	0.0060±0.0018	0.98	3.677	0.0107
11.8	4	2.278±0.015	0.0025±0.0021	0.79	2.606	0.0181
14.3	4	2.276±0.011	0.0060±0.0017	1.01	3.818	0.0067
16.1	4	2.261±0.012	0.0060±0.0018	0.99	1.860	0.0065
17.5	4	2.266±0.008	0.0054±0.0014	0.92	3.216	0.0035
19.6	4	2.241±0.019	0.0076±0.0030	0.93	2.413	0.0234
	5	2.241±0.019	0.0078±0.0030	0.81	1.008	0.0235
	6	2.242±0.019	0.0078±0.0030	0.73	1.037	0.0235
20.7	4	2.285±0.022	0.0138±0.0037	1.13	1.108	0.0215
	5	2.286±0.022	0.0139±0.0037	0.92	1.577	0.0215
	6	2.286±0.020	0.0139±0.0036	0.81	1.577	0.0215
21.9	4	2.327±0.031	0.0176±0.0055	1.35	1.366	0.0392
	5	2.321±0.022	0.0180±0.0037	1.12	1.262	0.0200
	6	2.321±0.023	0.0181±0.0037	0.94	1.271	0.0200
24.6	6	2.374±0.016	0.0123±0.0023	0.91	3.341	0.0138
26.7	6	2.369±0.017	0.0109±0.0027	0.91	2.707	0.0140
28.8	6	2.361±0.010	0.0104±0.0015	0.96	3.456	0.0040

Table S2. Fitting results of the first shell Zn-S distance, σ^2, S_0^2, ΔE_0, and *R*-factor at selected pressures for ZnS nanoparticles.

P (GPa)	*N*	*Zn-S distance (Å)*	*σ^2 (Å²)*	S_0^2	*ΔE_0 (eV)*	*R-factor*
0	4	2.339±0.005	0.0061±0.0007	0.96	4.027	0.0043
2.2	4	2.326±0.014	0.0071±0.0021	0.98	3.001	0.0119
3.9	4	2.313±0.012	0.0039±0.0018	0.82	3.111	0.0167
6.1	4	2.284±0.010	0.0054±0.0016	0.92	2.198	0.0080
8.3	4	2.277±0.012	0.0058±0.0018	0.93	1.860	0.0117
10.5	4	2.269±0.013	0.0056±0.0019	0.93	2.255	0.0122
11.9	4	2.273±0.020	0.0084±0.0025	1.01	3.219	0.0170
	5	2.269±0.022	0.0102±0.0042	0.88	3.548	0.0242
	6	2.267±0.025	0.0113±0.0046	0.73	3.668	0.0258
13.6	4	2.250±0.009	0.0032±0.0013	0.79	1.696	0.0085
	5	2.250±0.009	0.0033±0.0012	0.71	2.145	0.0084
	6	2.251±0.008	0.0033±0.0012	0.63	2.145	0.0083
15.6	4	2.276±0.013	0.0076±0.0022	0.87	3.615	0.0069
	5	2.277±0.014	0.0077±0.0022	0.76	3.248	0.0070
	6	2.277±0.014	0.0077±0.0022	0.68	3.064	0.0071
17.0	4	2.269±0.017	0.0104±0.0025	0.93	1.358	0.0145
	5	2.266±0.013	0.0105±0.0020	0.78	1.456	0.0119
	6	2.266±0.013	0.0105±0.0019	0.65	1.577	0.0121
18.7	4	2.344±0.017	0.0112±0.0029	0.95	2.842	0.0252
	5	2.319±0.018	0.0112±0.0030	0.77	3.505	0.0246
	6	2.320±0.018	0.0113±0.0030	0.64	3.477	0.0193
20.2	6	2.324±0.017	0.0102±0.0026	0.74	2.672	0.0189
22.2	6	2.310±0.012	0.0128±0.0019	0.78	0.576	0.0057
23.9	6	2.317±0.013	0.0102±0.0021	0.69	1.657	0.0098
25.6	6	2.309±0.016	0.0159±0.0010	1.00	0.610	0.0110
27.9	6	2.313±0.014	0.0095±0.0022	0.74	2.754	0.0107
30.2	6	2.299±0.014	0.0117±0.0022	0.80	1.024	0.0079