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α-Cu_2Se 精细结构的球差校正扫描透射电镜表征

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Characterization of α-Cu_2Se Fine Structure by Spherical-Aberration-Corrected Scanning Transmission Electron Microscope

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补充材料包括：8 种变体的原子分数坐标

以下表格是不同变体中原子的分数坐标：

表 S1　单胞 2L 变体 1 (空间群：$P\bar{1}$)中原子的分数坐标

Table S1　Atomic fractional coordinates of variate 1 of unit cell 2L (space group: $P\bar{1}$).

Atom	*x*	*y*	*z*
Cu1	0.209	0.084	0.272
Cu2	0.462	0.462	0.288
Cu3	0.165	0.659	0.790
Cu4	0.887	0.235	0.772
Cu5	0.805	0.716	0.284
Cu6	0.439	0.937	0.789
Cu7	0.860	0.014	0.104
Cu8	0.526	0.204	0.628
Cu9	0.486	0.723	0.171
Cu10	0.174	0.373	0.168
Cu11	0.846	0.541	0.638
Cu12	0.162	0.901	0.665
Se1	0.506	0.364	0.118
Se2	0.184	0.028	0.096
Se3	0.848	0.199	0.596
Se4	0.844	0.691	0.118
Se5	0.510	0.870	0.618
Se6	0.179	0.542	0.618

表 S2　单胞 2R 变体 1 (空间群：$P\bar{1}$)中原子的分数坐标

Table S2　Atomic fractional coordinates of variate 1 of unit cell 2R (space group: $P\bar{1}$).

Atom	*x*	*y*	*z*
Cu1	0.522	0.282	0.285
Cu2	0.376	0.064	0.790
Cu3	0.292	0.919	0.274
Cu4	0.934	0.527	0.289
Cu5	0.828	0.335	0.791
Cu6	0.124	0.766	0.774
Cu7	0.541	0.631	0.169
Cu8	0.382	0.462	0.637
Cu9	0.207	0.279	0.172
Cu10	0.061	0.101	0.667
Cu11	0.863	0.993	0.101
Cu12	0.720	0.802	0.621
Se1	0.524	0.316	0.118
Se2	0.374	0.134	0.618
Se3	0.864	0.638	0.118
Se4	0.718	0.458	0.618
Se5	0.206	0.977	0.096
Se6	0.042	0.806	0.596

表 S3　单胞 2L 变体 2 (空间群：*P*1)中原子的分数坐标

Table S3　Atomic fractional coordinates of variate 2 of unit cell 2L (space group: *P*1).

Atom	*x*	*y*	*z*
Cu1	0.213	0.090	0.272
Cu2	0.435	0.482	0.283
Cu3	0.168	0.657	0.790
Cu4	0.883	0.232	0.773
Cu5	0.825	0.722	0.287
Cu6	0.436	0.942	0.790
Cu7	0.846	0.042	0.098
Cu8	0.524	0.207	0.632
Cu9	0.494	0.732	0.171
Cu10	0.163	0.384	0.171
Cu11	0.845	0.538	0.631
Cu12	0.162	0.900	0.667
Cu13	0.565	0.073	0.212
Cu14	0.819	0.368	0.224
Cu15	0.539	0.544	0.711
Cu16	0.186	0.289	0.716
Cu17	0.100	0.801	0.212
Cu18	0.792	0.911	0.727
Cu19	0.153	0.454	0.369
Cu20	0.829	0.126	0.338
Cu21	0.514	0.275	0.829
Cu22	0.496	0.789	0.369
Cu23	0.139	0.985	0.897
Cu24	0.826	0.624	0.829
Se1	0.504	0.374	0.118
Se2	0.185	0.031	0.096
Se3	0.849	0.193	0.596
Se4	0.838	0.701	0.118
Se5	0.508	0.870	0.618
Se6	0.179	0.542	0.618
Se7	0.495	0.131	0.382
Se8	0.155	0.307	0.882
Se9	0.156	0.802	0.382
Se10	0.825	0.469	0.404
Se11	0.495	0.633	0.882
Se12	0.815	0.969	0.904

表 S4　单胞 2R 变体 2 (空间群：*P*1)中原子的分数坐标

Table S4　Atomic fractional coordinates of variate 2 of unit cell 2R (space group: *P*1).

Atom	*x*	*y*	*z*
Cu1	0.523	0.300	0.284
Cu2	0.377	0.061	0.790
Cu3	0.310	0.908	0.275
Cu4	0.944	0.506	0.285
Cu5	0.832	0.339	0.791
Cu6	0.114	0.776	0.776
Cu7	0.552	0.620	0.174
Cu8	0.380	0.465	0.625
Cu9	0.220	0.271	0.171
Cu10	0.061	0.102	0.667
Cu11	0.871	0.973	0.090
Cu12	0.724	0.798	0.628
Cu13	0.182	0.655	0.210
Cu14	0.895	0.196	0.213
Cu15	0.703	0.092	0.724
Cu16	0.640	0.937	0.212
Cu17	0.473	0.710	0.715
Cu18	0.081	0.470	0.711
Cu19	0.304	0.191	0.380
Cu20	0.630	0.531	0.371
Cu21	0.454	0.378	0.826
Cu22	0.133	0.011	0.901
Cu23	0.973	0.855	0.338
Cu24	0.790	0.726	0.828
Se1	0.530	0.309	0.118
Se2	0.373	0.131	0.618
Se3	0.870	0.629	0.118
Se4	0.721	0.457	0.618
Se5	0.213	0.970	0.096
Se6	0.039	0.811	0.596
Se7	0.311	0.519	0.404
Se8	0.977	0.179	0.382
Se9	0.787	0.030	0.904
Se10	0.646	0.853	0.382
Se11	0.473	0.688	0.882
Se12	0.134	0.368	0.882

表 S5　单胞 2L 变体 3 (空间群：*P*1)中原子的分数坐标

Table S5　Atomic fractional coordinates of variate 3 of unit cell 2L (space group: *P*1).

Atom	*x*	*y*	*z*
Cu1	0.209	0.089	0.273
Cu2	0.461	0.457	0.288
Cu3	0.182	0.630	0.776
Cu4	0.899	0.199	0.788
Cu5	0.814	0.711	0.284
Cu6	0.435	0.927	0.788
Cu7	0.861	0.015	0.103
Cu8	0.504	0.212	0.631
Cu9	0.487	0.725	0.171
Cu10	0.174	0.376	0.171
Cu11	0.847	0.546	0.631
Cu12	0.171	0.874	0.663
Cu13	0.564	0.059	0.210
Cu14	0.833	0.342	0.210
Cu15	0.565	0.519	0.717
Cu16	0.174	0.278	0.713
Cu17	0.117	0.769	0.227
Cu18	0.787	0.909	0.728
Cu19	0.156	0.462	0.369
Cu20	0.838	0.100	0.334
Cu21	0.506	0.268	0.829
Cu22	0.476	0.793	0.368
Cu23	0.154	0.957	0.902
Cu24	0.837	0.616	0.829
Se1	0.506	0.367	0.118
Se2	0.185	0.032	0.096
Se3	0.844	0.198	0.618
Se4	0.845	0.693	0.118
Se5	0.505	0.869	0.618
Se6	0.174	0.531	0.596
Se7	0.492	0.130	0.382
Se8	0.162	0.298	0.882
Se9	0.151	0.807	0.404
Se10	0.821	0.459	0.382
Se11	0.496	0.625	0.882
Se12	0.815	0.968	0.904

表 S6　单胞 2R 变体 3 (空间群：*P*1)中原子的分数坐标

Table S6　Atomic fractional coordinates of variate 3 of unit cell 2R (space group: *P*1).

Atom	*x*	*y*	*z*
Cu1	0.526	0.292	0.284
Cu2	0.359	0.073	0.788
Cu3	0.300	0.911	0.273
Cu4	0.918	0.543	0.288
Cu5	0.812	0.366	0.777
Cu6	0.097	0.802	0.788
Cu7	0.551	0.624	0.172
Cu8	0.389	0.456	0.631
Cu9	0.213	0.276	0.170
Cu10	0.042	0.129	0.662
Cu11	0.876	0.987	0.102
Cu12	0.713	0.791	0.630
Cu13	0.174	0.660	0.210
Cu14	0.888	0.230	0.227
Cu15	0.693	0.091	0.728
Cu16	0.625	0.942	0.211
Cu17	0.453	0.721	0.713
Cu18	0.080	0.483	0.717
Cu19	0.271	0.207	0.368
Cu20	0.619	0.539	0.371
Cu21	0.451	0.384	0.829
Cu22	0.112	0.040	0.903
Cu23	0.940	0.900	0.334
Cu24	0.773	0.731	0.829
Se1	0.539	0.307	0.118
Se2	0.372	0.132	0.618
Se3	0.874	0.633	0.118
Se4	0.703	0.470	0.596
Se5	0.218	0.968	0.096
Se6	0.040	0.804	0.618
Se7	0.281	0.543	0.382
Se8	0.959	0.194	0.404
Se9	0.782	0.032	0.904
Se10	0.623	0.873	0.382
Se11	0.459	0.701	0.882
Se12	0.120	0.374	0.882

表 S7　单胞 4L (空间群：$P\bar{1}$)中原子的分数坐标

Table S7　Atomic fractional coordinates of of unit cell 4L (space group: $P\bar{1}$).

Atom	*x*	*y*	*z*
Cu1	0.441	0.418	0.149
Cu2	0.170	0.046	0.137
Cu3	0.695	0.122	0.390
Cu4	0.323	0.217	0.633
Cu5	0.750	0.715	0.149
Cu6	0.305	0.806	0.396
Cu7	0.071	0.455	0.383
Cu8	0.572	0.543	0.651
Cu9	0.174	0.659	0.896
Cu10	0.895	0.285	0.886
Cu11	0.959	0.869	0.648
Cu12	0.472	0.958	0.895
Cu13	0.861	0.009	0.061
Cu14	0.403	0.125	0.328
Cu15	0.474	0.704	0.089
Cu16	0.173	0.340	0.079
Cu17	0.764	0.447	0.314
Cu18	0.304	0.527	0.587
Cu19	0.023	0.196	0.569
Cu20	0.586	0.250	0.811
Cu21	0.035	0.774	0.334
Cu22	0.643	0.884	0.575
Cu23	0.901	0.584	0.824
Cu24	0.200	0.943	0.838
Se1	0.508	0.353	0.064
Se2	0.193	0.005	0.050
Se3	0.752	0.107	0.303
Se4	0.340	0.203	0.546
Se5	0.846	0.674	0.064
Se6	0.417	0.778	0.311
Se7	0.099	0.432	0.296
Se8	0.661	0.533	0.564
Se9	0.917	0.246	0.800
Se10	0.002	0.862	0.561
Se11	0.570	0.918	0.811
Se12	0.238	0.593	0.811

表 S8　单胞 4R (空间群：$P\bar{1}$)中原子的分数坐标

Table S8　Atomic fractional coordinates of of unit cell 4R (space group: $P\bar{1}$).

Atom	*x*	*y*	*z*
Cu1	0.464	0.278	0.149
Cu2	0.115	0.192	0.396
Cu3	0.214	0.966	0.139
Cu4	0.895	0.549	0.150
Cu5	0.534	0.542	0.384
Cu6	0.108	0.453	0.651
Cu7	0.821	0.139	0.648
Cu8	0.424	0.051	0.895
Cu9	0.818	0.885	0.391
Cu10	0.537	0.778	0.634
Cu11	0.181	0.722	0.887
Cu12	0.839	0.324	0.897
Cu13	0.512	0.662	0.076
Cu14	0.185	0.296	0.088
Cu15	0.817	0.226	0.335
Cu16	0.522	0.116	0.575
Cu17	0.861	0.995	0.056
Cu18	0.531	0.876	0.328
Cu19	0.213	0.555	0.309
Cu20	0.827	0.472	0.589
Cu21	0.472	0.420	0.829
Cu22	0.140	0.063	0.838
Cu23	0.214	0.804	0.566
Cu24	0.815	0.765	0.800
Se1	0.515	0.328	0.064
Se2	0.861	0.644	0.064
Se3	0.536	0.567	0.296
Se4	0.197	0.221	0.311
Se5	0.858	0.141	0.561
Se6	0.473	0.092	0.811
Se7	0.193	0.998	0.050
Se8	0.860	0.897	0.303
Se9	0.541	0.795	0.546
Se10	0.187	0.467	0.564
Se11	0.817	0.409	0.811
Se12	0.149	0.760	0.800