

The effect of Fe vacancies and Cu adhesion on the magnetic properties of Fe₃GeTe₂

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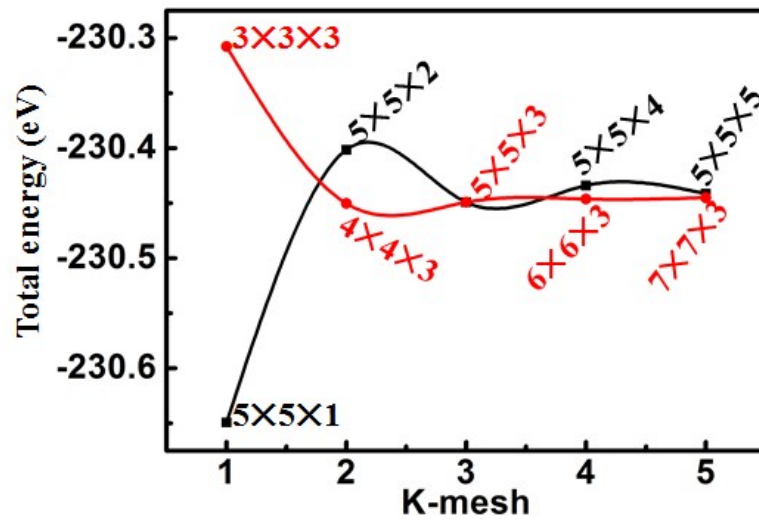


Fig. S1. Total energy of Fe_3GeTe_2 with different K-meshes.

Table S1. Coordinates and Bader charge distributions of perfect Fe₃GeTe₂

Atoms	x	y	z	Bader Charge
Fe ^{II}	1.155	2.000	12.340	8.091
Fe ^{II}	2.309	0.000	4.113	8.091
Fe ^I	0.000	0.000	11.102	7.674
Fe ^I	3.464	2.000	11.102	7.674
Fe ^I	0.000	4.000	11.102	7.674
Fe ^I	0.000	0.000	2.875	7.674
Fe ^I	3.464	2.000	2.875	7.674
Fe ^I	0.000	4.000	2.875	7.674
Fe ^I	0.000	0.000	5.352	7.632
Fe ^I	3.464	2.000	5.352	7.632
Fe ^I	0.000	4.000	5.352	7.632
Fe ^I	0.000	0.000	13.579	7.632
Fe ^I	3.464	2.000	13.579	7.632
Fe ^I	0.000	4.000	13.579	7.632
Fe ^{II}	4.619	0.000	12.340	8.091
Fe ^{II}	-2.309	4.000	12.340	8.091
Fe ^{II}	-1.155	2.000	4.113	8.091
Fe ^{II}	2.309	4.000	4.113	8.091
Ge	2.309	0.000	12.340	4.014
Ge	-1.155	2.000	12.340	4.014
Ge	2.309	4.000	12.340	4.014
Ge	4.619	0.000	4.113	4.014
Ge	1.155	2.000	4.113	4.014
Ge	-2.309	4.000	4.113	4.014
Te	4.619	0.000	9.751	6.295
Te	1.155	2.000	9.751	6.295
Te	-2.309	4.000	9.751	6.295
Te	2.309	0.000	1.524	6.295
Te	-1.155	2.000	1.524	6.295
Te	2.309	4.000	1.524	6.295
Te	2.309	0.000	6.703	6.295
Te	-1.155	2.000	6.703	6.295
Te	2.309	4.000	6.703	6.295
Te	4.619	0.000	14.930	6.295
Te	1.155	2.000	14.930	6.295
Te	-2.309	4.000	14.930	6.295

Table S2. Coordinates and Bader charge distributions of Fe₃GeTe₂ with 5.56% Fe^{II} vacancy.

Atoms	x	y	z	Bader Charge
Fe ^{II}	2.288	0.001	4.097	8.093
Fe ^I	3.413	5.911	11.090	7.762
Fe ^I	3.473	1.982	11.090	7.757
Fe ^I	-0.020	3.998	11.090	7.757
Fe ^I	3.430	5.941	2.851	7.687
Fe ^I	3.438	1.982	2.851	7.676
Fe ^I	-0.003	3.968	2.851	7.676
Fe ^I	3.430	5.941	5.343	7.649
Fe ^I	3.438	1.982	5.343	7.638
Fe ^I	-0.003	3.968	5.343	7.638
Fe ^I	3.413	5.911	13.492	7.712
Fe ^I	3.473	1.982	13.492	7.706
Fe ^I	-0.020	3.998	13.492	7.706
Fe ^{II}	4.577	0.000	12.291	7.977
Fe ^{II}	-2.288	3.964	12.291	7.977
Fe ^{II}	-1.143	1.982	4.097	8.093
Fe ^{II}	2.288	3.963	4.097	8.093
Ge	2.165	0.213	12.291	3.999
Ge	-0.898	1.982	12.291	3.999
Ge	2.165	3.751	12.291	3.994
Ge	4.577	0.000	4.097	4.002
Ge	1.144	1.982	4.097	3.983
Ge	-2.288	3.964	4.097	4.002
Te	4.577	0.000	9.718	6.276
Te	1.144	1.982	9.783	6.312
Te	-2.288	3.964	9.718	6.276
Te	2.279	0.016	1.490	6.283
Te	-1.126	1.982	1.490	6.283
Te	2.279	3.948	1.490	6.283
Te	2.279	0.016	6.704	6.283
Te	-1.126	1.982	6.704	6.283
Te	2.279	3.948	6.704	6.283
Te	4.577	0.000	14.865	6.276
Te	1.144	1.982	14.799	6.312
Te	-2.288	3.964	14.865	6.276

Table S3. Coordinates and Bader charge distributions of Fe₃GeTe₂ with 11.11% Fe^{II} vacancy.

Agtoms	x	y	z	Bader Charge
Fe ^I	3.354	5.828	11.092	7.788
Fe ^I	3.418	1.955	11.092	7.784
Fe ^I	-0.020	3.938	11.091	7.778
Fe ^I	3.338	5.855	2.892	7.787
Fe ^I	3.403	1.983	2.892	7.786
Fe ^I	0.014	3.878	2.890	7.778
Fe ^I	3.338	5.855	5.309	7.740
Fe ^I	3.403	1.983	5.309	7.740
Fe ^I	0.014	3.878	5.310	7.732
Fe ^I	3.354	5.828	13.509	7.742
Fe ^I	3.418	1.955	13.509	7.738
Fe ^I	-0.020	3.938	13.511	7.732
Fe ^{II}	1.122	5.859	12.301	7.986
Fe ^{II}	-2.255	3.909	12.301	7.985
Fe ^{II}	-1.128	1.957	4.100	7.983
Fe ^{II}	2.249	3.907	4.100	7.986
Ge	2.131	0.212	12.301	3.981
Ge	-0.884	1.952	12.301	3.988
Ge	2.132	3.693	12.301	3.981
Ge	4.264	-0.001	4.100	3.987
Ge	1.249	1.740	4.100	3.978
Ge	-2.138	4.123	4.100	3.984
Te	4.497	0.010	9.717	6.246
Te	1.132	1.941	9.774	6.266
Te	-2.263	3.926	9.717	6.247
Te	2.248	0.010	1.574	6.265
Te	-1.117	1.942	1.516	6.249
Te	2.257	3.890	1.516	6.246
Te	2.248	0.010	6.627	6.265
Te	-1.117	1.942	6.684	6.249
Te	2.257	3.890	6.684	6.246
Te	4.497	0.010	14.884	6.246
Te	1.132	1.941	14.827	6.266
Te	-2.263	3.926	14.884	6.247

Table S4. Coordinates and Bader charge distributions of perfect Fe₃GeTe₂/Cu interlayer.

Atoms	x	y	z	Bader Charge
Fe ^I	3.376	5.836	15.359	7.713
Fe ^I	3.379	1.938	15.351	7.688
Fe ^I	0.006	3.887	15.351	7.688
Fe ^I	3.364	5.837	6.856	7.800
Fe ^I	3.371	1.923	6.842	7.785
Fe ^I	0.001	3.889	6.843	7.784
Fe ^I	3.373	5.832	9.431	7.645
Fe ^I	3.372	1.934	9.424	7.646
Fe ^I	0.003	3.883	9.424	7.650
Fe ^I	3.377	5.818	17.925	7.756
Fe ^I	3.384	1.940	17.923	7.742
Fe ^I	-0.006	3.887	17.922	7.744
Fe ^{II}	1.123	5.833	16.447	8.209
Fe ^{II}	4.506	3.880	16.438	8.235
Fe ^{II}	5.621	1.938	8.333	8.187
Fe ^{II}	2.249	3.885	8.333	8.186
Fe ^{II}	1.131	1.944	16.457	8.233
Fe ^{II}	-1.129	5.827	8.336	8.182
Ge	-1.127	5.831	16.754	3.969
Ge	5.627	1.933	16.763	3.968
Ge	2.260	3.892	16.756	3.965
Ge	1.120	5.832	8.025	3.974
Ge	1.125	1.937	8.022	3.973
Ge	4.494	3.880	8.018	3.970
Te	1.145	5.830	13.925	6.185
Te	1.125	1.925	13.931	6.180
Te	-2.256	3.907	13.920	6.183
Te	-1.145	5.829	5.436	6.206
Te	5.619	1.921	5.435	6.204
Te	2.253	3.902	5.450	6.201
Te	-1.115	5.830	10.862	6.229
Te	5.619	1.942	10.859	6.223
Te	2.254	3.878	10.863	6.229
Te	1.126	5.821	19.361	6.256
Te	1.123	1.922	19.253	6.115
Te	4.494	3.881	19.392	6.228
Cu	0.615	4.448	21.698	10.989
Cu	3.495	1.112	21.697	10.973
Cu	3.014	3.619	21.711	10.993

Cu	5.910	0.284	21.701	10.978
Cu	-1.316	2.774	21.713	10.995
Cu	-1.791	5.290	21.711	10.989
Cu	2.065	0.821	23.775	10.996
Cu	1.586	3.354	23.775	10.979
Cu	4.462	0.000	23.767	10.980
Cu	3.977	2.498	23.753	10.990
Cu	3.501	5.021	23.751	10.982
Cu	-0.370	1.670	23.777	10.989
Cu	-0.824	4.169	23.752	10.986
Cu	1.089	1.948	21.793	11.122
Cu	0.634	4.445	3.028	10.980
Cu	3.489	1.104	3.030	10.979
Cu	3.035	3.619	2.973	11.032
Cu	5.911	0.297	3.027	10.986
Cu	-1.317	2.791	2.972	11.033
Cu	-1.797	5.274	2.969	11.027
Cu	-0.340	5.556	0.950	10.982
Cu	2.546	2.218	0.947	10.982
Cu	2.062	4.745	0.950	10.986
Cu	4.935	1.386	0.951	10.988
Cu	4.466	3.894	0.924	10.990
Cu	0.605	0.555	0.946	10.982
Cu	1.094	1.948	2.962	10.996
Cu	0.136	3.073	0.945	10.983

Table S5. Coordinates and Bader charge distributions of Fe₃GeTe₂/Cu interlayer with 5.56% Fe^{II} vacancy.

Atoms	x	y	z	Bader Charge
Fe ^I	3.341	5.784	15.351	7.840
Fe ^I	3.422	1.923	15.336	7.836
Fe ^I	-0.020	3.917	15.342	7.833
Fe ^I	3.358	5.827	6.835	7.797
Fe ^I	3.364	1.918	6.823	7.789
Fe ^I	0.001	3.882	6.821	7.782
Fe ^I	3.364	5.825	9.420	7.651
Fe ^I	3.369	1.926	9.417	7.642
Fe ^I	-0.001	3.878	9.415	7.643
Fe ^I	3.333	5.755	17.784	7.758
Fe ^I	3.426	1.935	17.774	7.751
Fe ^I	-0.046	3.929	17.779	7.742
Fe ^{II}	1.122	5.813	16.505	8.028
Fe ^{II}	4.485	3.875	16.507	8.022
Fe ^{II}	5.608	1.938	8.336	8.153
Fe ^{II}	2.246	3.876	8.312	8.193
Fe ^{II}	-1.125	5.819	8.338	8.146
Ge	2.120	0.198	16.571	3.988
Ge	-0.885	1.932	16.572	3.987
Ge	2.122	3.658	16.556	3.962
Ge	1.120	5.820	7.999	3.971
Ge	1.121	1.934	7.985	3.966
Ge	4.486	3.877	7.987	3.963
Te	1.140	5.814	13.907	6.203
Te	1.121	1.923	14.056	6.230
Te	4.484	3.886	13.920	6.192
Te	-1.138	5.814	5.414	6.192
Te	5.607	1.915	5.414	6.193
Te	2.247	3.891	5.425	6.192
Te	-1.137	5.820	10.871	6.277
Te	-1.106	1.932	10.871	6.275
Te	2.250	3.870	10.836	6.245
Te	1.114	5.817	19.239	6.267
Te	1.121	1.934	19.076	6.242
Te	4.466	3.867	19.266	6.268
Cu	0.622	4.435	21.579	10.987
Cu	3.496	1.112	21.580	10.978
Cu	3.014	3.609	21.590	10.996
Cu	5.910	0.283	21.579	10.979
Cu	-1.301	2.768	21.589	10.994
Cu	-1.777	5.280	21.589	10.989

Cu	2.060	0.826	23.646	10.987
Cu	1.585	3.336	23.646	10.983
Cu	4.459	0.000	23.644	10.980
Cu	3.976	2.493	23.631	10.994
Cu	3.498	5.007	23.630	10.983
Cu	-0.355	1.668	23.647	10.985
Cu	-0.818	4.161	23.632	10.988
Cu	1.097	1.943	21.621	11.026
Cu	0.627	4.435	3.024	10.977
Cu	3.475	1.100	3.026	10.974
Cu	3.024	3.608	2.957	11.032
Cu	5.891	0.295	3.020	10.987
Cu	-1.319	2.784	2.960	11.029
Cu	-1.800	5.260	2.957	11.027
Cu	-0.340	5.545	0.936	10.985
Cu	2.540	2.209	0.937	10.983
Cu	2.057	4.732	0.936	10.987
Cu	4.925	1.383	0.937	10.985
Cu	4.457	3.885	0.912	10.989
Cu	0.601	0.556	0.935	10.985
Cu	1.086	1.943	2.959	11.001
Cu	0.138	3.067	0.936	10.990

Table S6. Coordinates and Bader charge distributions of Fe₃GeTe₂/Cu interlayer with 11.11% Fe^{II} vacancy.

Atoms	x	y	z	Bader Charge
Fe ^I	3.332	5.769	15.218	7.791
Fe ^I	3.379	1.923	15.215	7.775
Fe ^I	-0.016	3.887	15.215	7.775
Fe ^I	3.359	5.739	6.861	7.812
Fe ^I	3.285	1.913	6.863	7.819
Fe ^I	0.037	3.910	6.858	7.815
Fe ^I	3.369	5.733	9.327	7.800
Fe ^I	3.291	1.910	9.327	7.793
Fe ^I	0.033	3.892	9.325	7.800
Fe ^I	3.304	5.711	17.675	7.824
Fe ^I	3.416	1.925	17.674	7.830
Fe ^I	-0.049	3.920	17.673	7.826
Fe ^{II}	1.113	5.782	16.387	8.029
Fe ^{II}	4.455	3.851	16.384	8.026
Fe ^{II}	2.240	3.848	8.152	8.018
Fe ^{II}	-1.122	5.775	8.156	8.038
Ge	2.103	0.205	16.465	3.980
Ge	-0.870	1.919	16.466	3.974
Ge	2.101	3.635	16.453	3.967
Ge	4.583	0.207	8.090	3.970
Ge	0.857	1.920	8.082	3.985
Ge	4.597	3.617	8.087	3.977
Te	4.474	0.004	13.800	6.220
Te	1.113	1.931	13.876	6.216
Te	-2.232	3.867	13.799	6.221
Te	-1.112	5.786	5.430	6.229
Te	5.565	1.922	5.489	6.231
Te	2.225	3.855	5.430	6.230
Te	-1.115	5.777	10.759	6.170
Te	-1.106	1.917	10.634	6.215
Te	2.234	3.842	10.755	6.179
Te	1.112	5.787	19.135	6.227
Te	1.111	1.925	18.960	6.136
Te	4.448	3.853	19.150	6.231
Cu	0.614	4.406	21.468	10.989
Cu	3.469	1.103	21.469	10.981
Cu	2.992	3.584	21.478	11.002
Cu	5.867	0.280	21.472	10.981
Cu	-1.298	2.751	21.477	10.997
Cu	-1.773	5.244	21.476	10.992
Cu	2.042	0.819	23.537	10.988

Cu	1.569	3.313	23.540	10.978
Cu	1.083	5.791	23.543	10.981
Cu	3.948	2.475	23.526	10.992
Cu	3.473	4.973	23.527	10.984
Cu	-0.355	1.656	23.541	10.992
Cu	-0.816	4.132	23.526	10.988
Cu	1.085	1.930	21.505	11.108
Cu	0.621	4.404	3.037	10.980
Cu	3.460	1.090	3.041	10.977
Cu	3.009	3.577	2.975	11.038
Cu	5.858	0.288	3.055	10.979
Cu	-1.307	2.756	3.017	11.019
Cu	-1.789	5.219	2.982	11.031
Cu	-0.343	5.509	0.957	10.988
Cu	2.520	2.194	0.955	10.990
Cu	2.043	4.700	0.958	10.983
Cu	4.898	1.374	0.965	10.979
Cu	4.432	3.852	0.937	10.990
Cu	0.598	0.551	0.960	10.983
Cu	1.081	1.925	2.992	10.999
Cu	0.132	3.042	0.963	10.982
