Supplementary material for manuscript:

Electronic structure and magnetic properties of the graphene/Fe/Ni(111) intercalation-like system

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TABLE I: Results for the atomic structure of the three graphene/FM interface models and for the clean FM surface: d_0 is the distance between the graphene overlayer and the interface FM layer (the two values for the two nonequivalent carbon atoms are indicated); d_1 is the distance between the interface FM layer and the second FM layer; d_2 is the distance between the second and third FM layers; ΔE is the energy difference between the energy calculated for the different slabs and the energy calculated for the most stable geometry; m_{FM} is the interface/surface FM spin magnetic moment (the two values for the *sp* and *d* magnetizations are indicated); m_{C} is the interface carbon spin magnetic moment (the two values for the two nonequivalent carbon atoms are indicated).

	FM	Structure of the graphene/FM interface		
	Ni(111)	*top-fcc*	*top-hcp*	*fcc-hcp*
d_0 (Å)		2.135/2.133	2.145/2.146	3.540/3.540
d_1 (Å)	2.005	2.020	2.020	2.020
d_2 (Å)	2.031	2.017	2.015	2.036
ΔE (eV)		0.000	0.049	0.054
m_{FM} (μ_B)	−0.030/0.710	−0.025/0.543	−0.026/0.514	−0.029/0.669
m_{C} (μ_B)		−0.019/0.031	−0.019/0.027	0.000/0.000
	1ML Fe/Ni(111)	*TOP-FCC*	*TOP-HCP*	*FCC-HCP*
d_0 (Å)		2.117/2.092	2.114/2.089	3.487/3.487
d_1 (Å)	2.039	2.029	2.019	2.028
d_2 (Å)	2.061	2.044	2.057	2.062
ΔE (eV)		0.021	0.000	0.104
m_{FM} (μ_B)	−0.028/2.622	−0.034/2.486	−0.035/2.469	−0.022/2.616
m_{C} (μ_B)		−0.048/0.040	−0.050/0.039	0.000/0.000

TABLE II: Binding energies (in eV) (positive sign for states below the Fermi level and negative sign for states above the Fermi level) of the interface hybrid states (I_i) extracted from the calculated band structures of the graphene/FM system at the K and M points (see text for details).

State	FM = Ni(111)		FM = 1ML Fe/Ni(111)	
	spin ↑	spin ↓	spin ↑	spin ↓
I_5	−3.20	−3.32	−3.56	−4.05
I_4	−0.12	−0.55	−0.28	−1.72
I_3	0.28	−0.16	0.26	−1.19
I_2	2.28	1.93	2.32	1.99
I_1	3.27	2.93	3.75	2.77

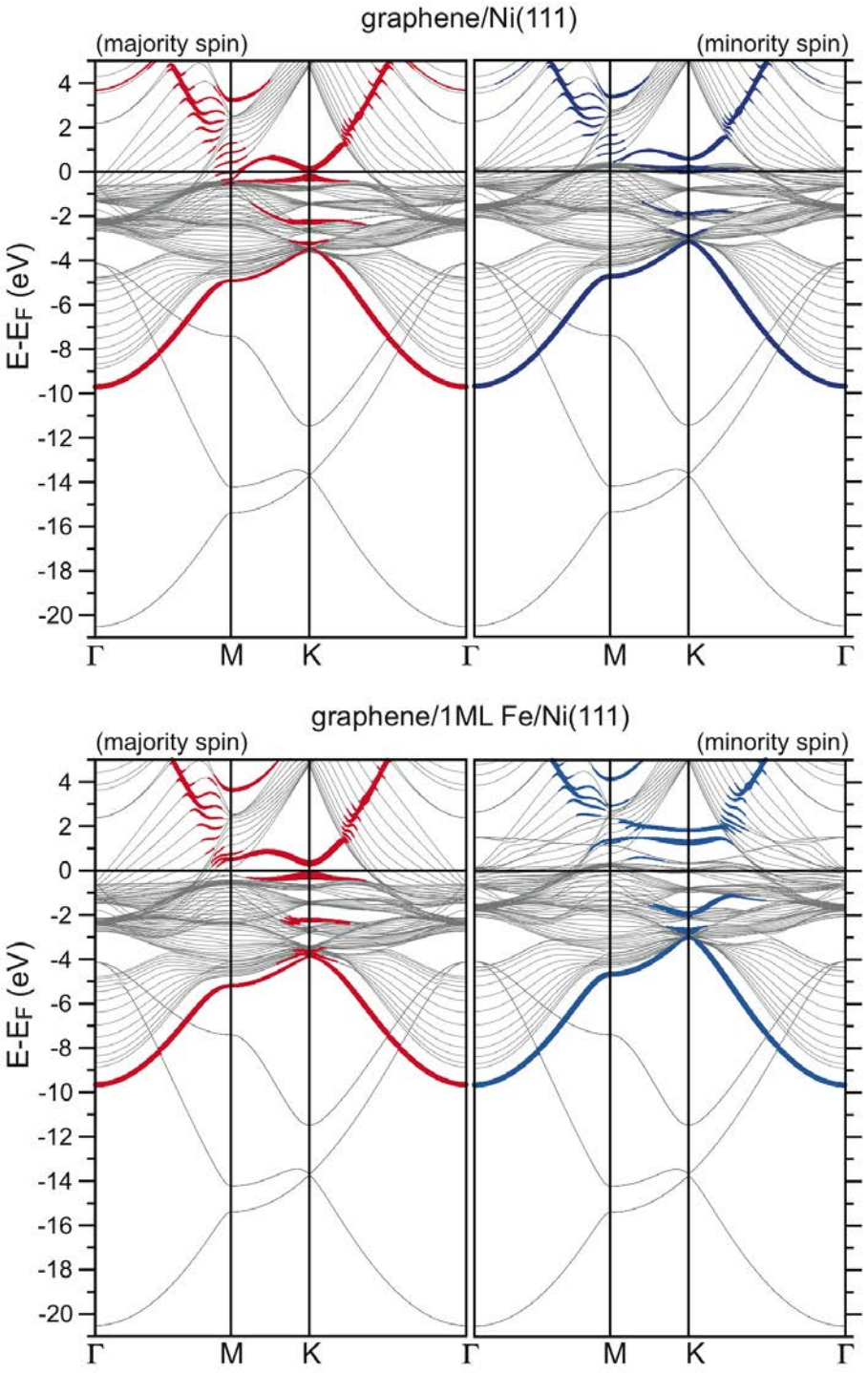

Fig. S1. Calculated majority and minority spin band structures of the graphene/Ni(111) and graphene/1 ML Fe(111)/Ni(111) interfaces for a most energetically favorable configurations. For the blue/red (thicker) lines, the carbon p_z character is used as a weighting factor.

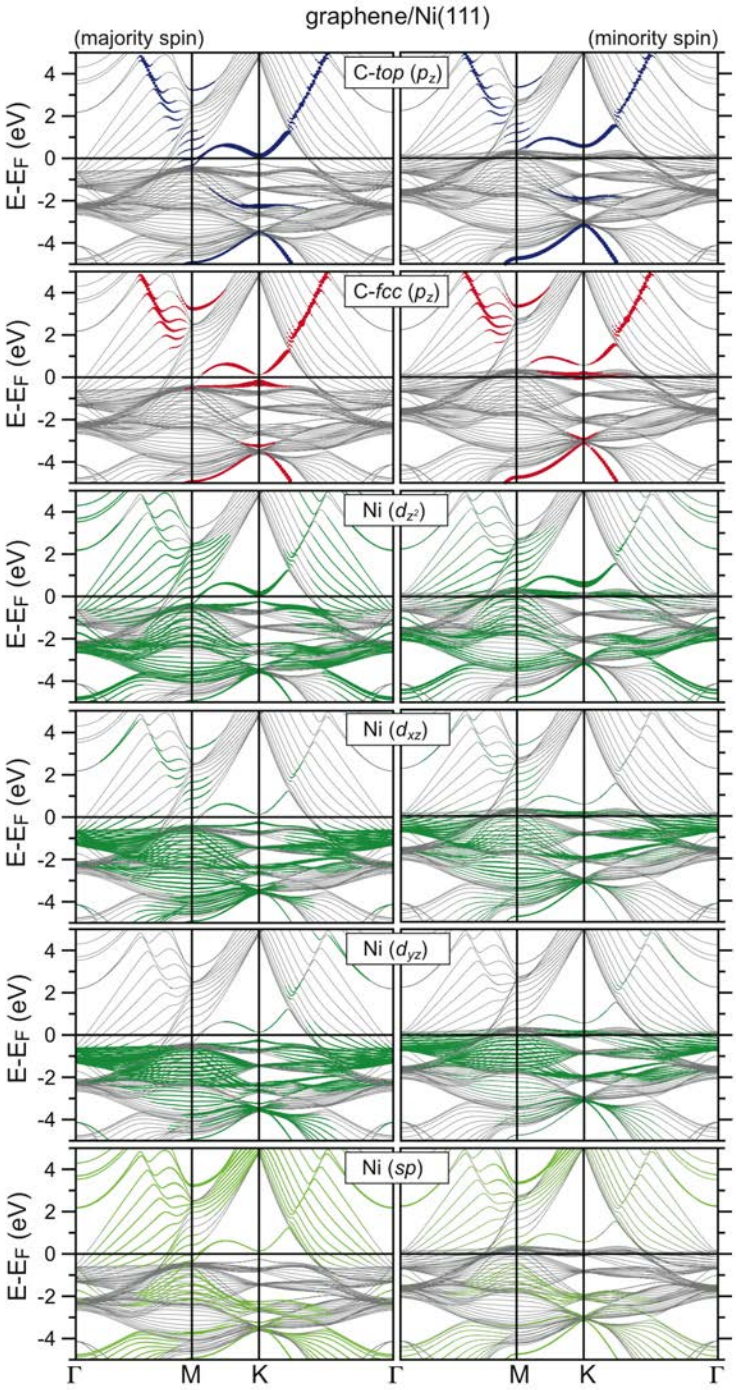

Fig. S2. Detailed analysis of the electronic structure of the graphene/Ni(111) system where the corresponding weights of Ni- and C-projected bands are shown by thick lines.

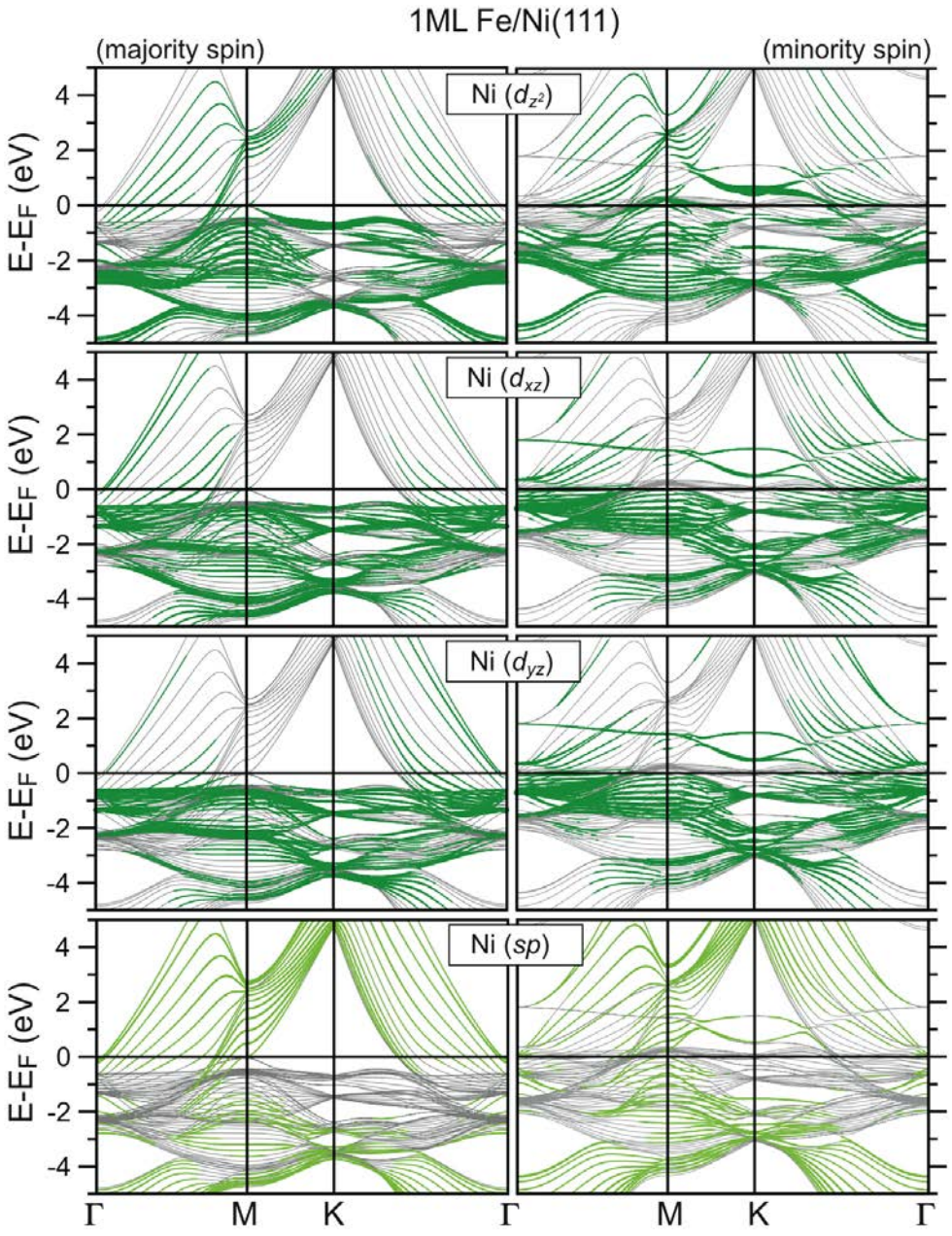

Fig. S3. Detailed analysis of the electronic structure of the 1 ML Fe/Ni(111) system where the corresponding weights of Ni-projected bands are shown by thick lines.

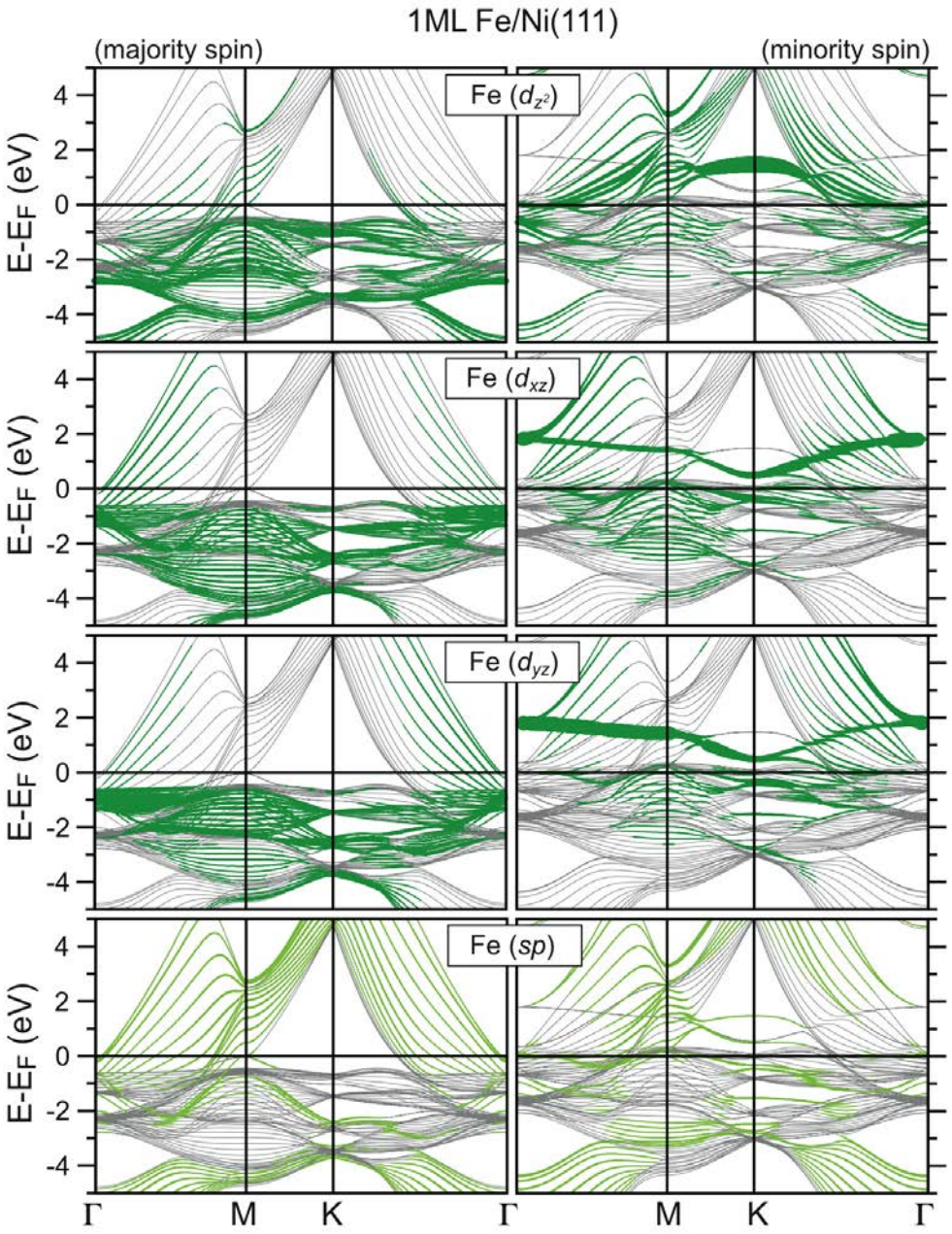

Fig. S4. Detailed analysis of the electronic structure of the 1 ML Fe/Ni(111) system where the corresponding weights of Fe-projected bands are shown by thick lines.

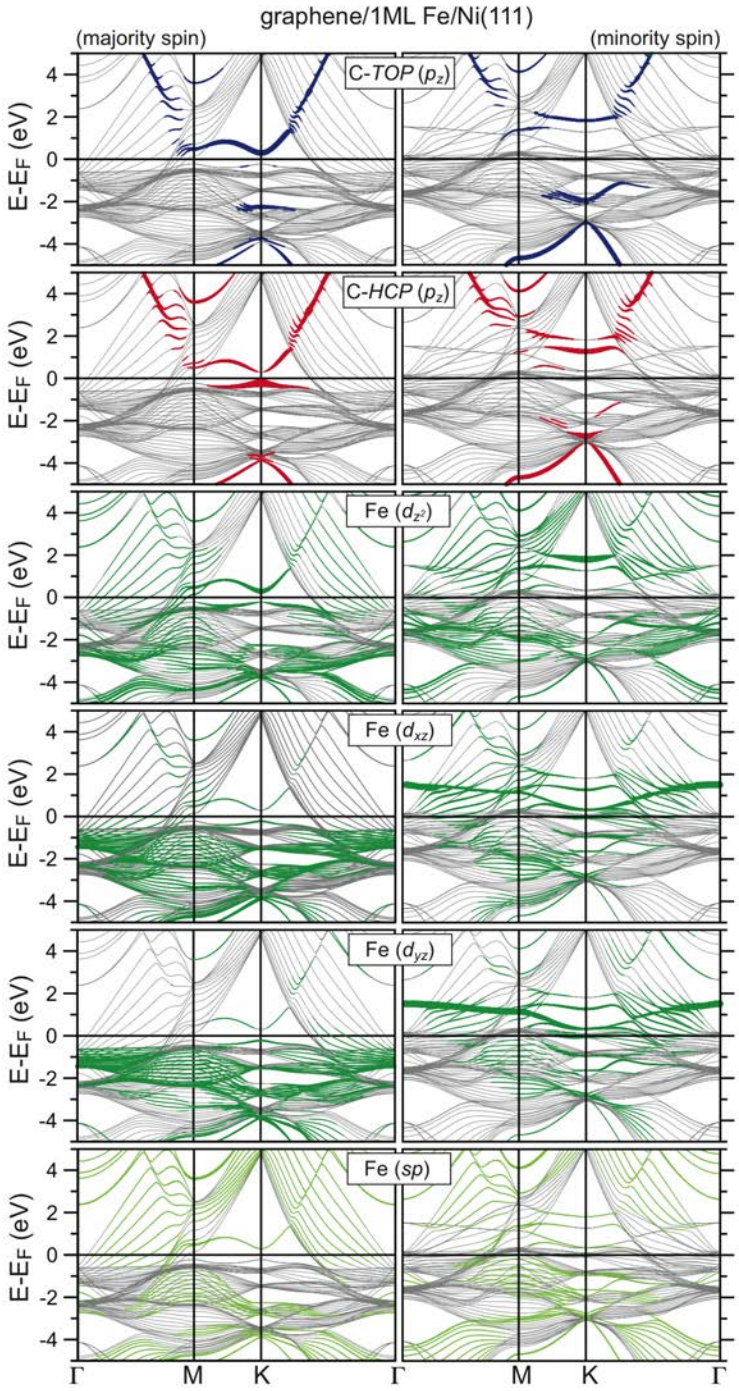

Fig. S5. Detailed analysis of the electronic structure of the graphene/1 ML Fe(111)/ Ni(111) system where the corresponding weights of Fe- and C-projected bands are shown by thick lines.