Supplementary information for the manuscript:

Electronic and Magnetic Properties of the Graphene-Y-Co(0001) Interfaces: Insights From the DFT Analysis

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Table S1: Results obtained for gr/Co(0001): ∆E (in eV/C-atom) is the relative total energy with respect to the energetically most favourable structure; $d_0$ (in Å) is the mean distance between the graphene overlayer and the interface substrate layer; $d_1$ (in Å) is the mean distance between the interface substrate layer and the second substrate layer; $m_C$ ($\mu_B$) is the interface C spin magnetic moment (two values for the nonequivalent carbon atoms are indicated); $m_{Co}$ ($\mu_B$) is the Co spin magnetic moment (two values are given for the interface/bulk atoms).

| Structure | ∆E | $d_0$ | $d_1$ | $m_C$ (µB) | $m_{Co}$ (µB) | Reference |
|-----------|-----|-------|-------|-------------|--------------|-----------|
| top-fcc   | 0.00 | 2.09  | 1.92  | 0.042/0.039 | 1.508/1.628  | Fig. S1a  |
| top-hcp   | 0.01 | 2.09  | 1.91  | 0.047/0.044 | 1.493/1.627  | Fig. S1b  |
| fcc-hcp   | 0.12 | 3.05  | 1.91  | −0.001/0.001| 1.693/1.631  | Fig. S1c  |
Table S2: Results obtained for gr/Y/Co(0001): $\Delta E$ (in eV/C-atom) is the relative total energy with respect to the energetically most favourable structure; $d_0$ (in Å) is the mean distance between the graphene overlayer and the interface substrate layer; $d_1$ (in Å) is the mean distance between the interface substrate layer and the second substrate layer; $d_2$ (in Å) is the mean distance between the second substrate layer and the third substrate layer; $m_{Co}(\mu_B)$ is the Co spin magnetic moment (two values are given for the interface/bulk atoms); $m_Y(\mu_B)$ is the Y spin magnetic moment.

| Structure       | $\Delta E$ | $d_0$ | $d_1$ | $d_2$ | $m_Y$  | $m_{Co}$ | Reference   |
|-----------------|------------|-------|-------|-------|--------|----------|-------------|
| gr/1 ML-Y/Co(0001) |            |       |       |       |        |          |             |
| FCC             | 0.00       | 2.55  | 2.61  | 1.93  | −0.094 | 1.537/1.642 | Fig. S5a   |
| HCP             | 0.11       | 2.58  | 2.53  | 1.93  | −0.126 | 1.423/1.638 | Fig. S5b   |
| TOP             | 0.18       | 2.57  | 2.89  | 1.94  | 0.088  | 1.521/1.640 | Fig. S5c   |
| gr/0.33 ML-Y/Co(0001) |          |       |       |       |        |          |             |
| FCC             | 0.06       | 2.40  | 2.24  | 1.94  | −0.181 | 1.443/1.618 | Fig. S5d   |
| HCP             | 0.00       | 2.28  | 2.31  | 1.95  | −0.112 | 1.499/1.620 | Fig. S5e   |
| TOP             | 0.03       | 2.41  | 2.27  | 1.99  | −0.192 | 1.265/1.620 | Fig. S5f   |
| gr/0.25 ML-Y/Co(0001) |          |       |       |       |        |          |             |
| FCC             | 0.03       | 2.53  | 2.16  | 1.96  | −0.230 | 1.404/1.599 | Fig. S5g   |
| HCP             | 0.00       | 2.32  | 2.19  | 1.95  | −0.182 | 1.443/1.633 | Fig. S5h   |
| TOP             | 0.01       | 2.45  | 2.18  | 1.96  | −0.198 | 1.583/1.598 | Fig. S5i   |
Table S3: Interface C spin magnetic moment (several values for the nonequivalent carbon atoms are indicated) of gr/Y/Co(0001).

| Structure     | $m_{C1}$ | $m_{C2}$ | $m_{C3}$ | Reference |
|---------------|----------|----------|----------|-----------|
| gr/1 ML-Y/Co(0001) |          |          |          |           |
| FCC           | −0.016   | 0.006    | -        | Fig. S5a |
| HCP           | −0.003   | −0.002   | -        | Fig. S5b |
| TOP           | −0.002   | −0.013   | -        | Fig. S5c |
| gr/0.33 ML-Y/Co(0001) |          |          |          |           |
| FCC           | 0.002    | −0.001   | 0.005    | Fig. S5d |
| HCP           | 0.005    | 0.010    | -        | Fig. S5e |
| TOP           | 0.015    | 0.006    | −0.004   | Fig. S5f |
| gr/0.25 ML-Y/Co(0001) |          |          |          |           |
| FCC           | −0.002   | −0.005   | 0.002    | Fig. S5g |
| HCP           | −0.001   | 0.001    | -        | Fig. S5h |
| TOP           | 0.002    | 0.001    | −0.015   | Fig. S5i |
Table S4: Layer resolved magnetic moments $\mu_i$ (in $\mu_B$) for Co-terminated and Y-terminated YCo$_2$(111) surfaces. The numbering of the layers starts at the surface Co layer (layer 1) which may be capped with one Y cap layer (layer 0). Subscripts $a$, $b$ label different sites as depicted in Fig. S10.

| Layer ($i$) | Atom type | Co-terminated $\mu_i$ | Y-terminated $\mu_i$ |
|------------|-----------|----------------------|---------------------|
| 0          | $Y_b$     | -                    | -0.305              |
| 1          | Co$_a$    | 1.203                | 1.183               |
| 2          | $Y_a$     | -0.299               | -0.219              |
| 3          | Co$_b$    | 0.985                | 0.630               |
| 4          | $Y_b$     | -0.166               | -0.119              |
| 5          | Co$_a$    | -0.063               | 0.056               |
| 6          | $Y_a$     | -0.011               | -0.014              |
| 7          | Co$_b$    | 0.164                | -0.195              |
| 8          | $Y_b$     | -0.013               | -0.009              |
| 9          | Co$_a$    | -0.020               | 0.048               |
Table S5: Results obtained for gr/1ML-YCo₂/Co(0001): $\Delta E$ (in eV/C-atom) is the relative total energy with respect to the energetically most favourable structure; $d_0$ (in Å) is the mean distance between the graphene overlayer and the interface substrate layer; $d_1$ (in Å) is the mean distance between the interface substrate layer and the second substrate layer; $d_2$ (in Å) is the mean distance between the second substrate layer and the third substrate layer; $d_3$ (in Å) is the mean distance between the third substrate layer and the fourth substrate layer; $m_{\text{Co}}$ ($\mu_B$) is the Co spin magnetic moment (two values are given for the interface/bulk atoms); $m_Y$ ($\mu_B$) is the Y spin magnetic moment.

| Structure | $\Delta E$ | $d_0$ | $d_1$ | $d_2$ | $d_3$ | $m_Y$ | $m_{\text{Co}}$ | Reference |
|-----------|------------|-------|-------|-------|-------|-------|--------------|-----------|
| Co-terminated YCo₂(111) |            |       |       |       |       |       |              |           |
| top-fcc   | 0.01       | 2.05  | 1.19  | 0.74  | 0.87  | $-0.282$ | 1.290/1.534 | Fig. S12a |
| top-hcp   | 0.00       | 2.01  | 1.16  | 0.77  | 0.87  | $-0.286$ | 1.268/1.534 | Fig. S12b |
| fcc-hcp   | 0.14       | 2.95  | 1.20  | 0.78  | 0.82  | $-0.372$ | 1.297/1.535 | Fig. S12c |
| Y-terminated YCo₂(111) |            |       |       |       |       |       |              |           |
| top-fcc   | 0.04       | 2.41  | 0.97  | 0.84  | 1.02  | $-0.235$ | 1.286/1.534 | Fig. S12d |
| top-hcp   | 0.04       | 2.46  | 0.92  | 0.86  | 1.01  | $-0.248$ | 1.344/1.534 | Fig. S12e |
| fcc-hcp   | 0.00       | 2.27  | 0.93  | 0.85  | 1.03  | $-0.254$ | 1.282/1.533 | Fig. S12f |
Table S6: Interface C spin magnetic moment (several values for the nonequivalent carbon atoms are indicated) of gr/1ML-YCo$_2$/Co(0001).

| Structure      | $m_{C1}$ | $m_{C2}$ | $m_{C3}$ | Reference  |
|----------------|----------|----------|----------|------------|
| Co-terminated YCo$_2$(111) |          |          |          |            |
| top-fcc        | -0.033   | 0.023    | -0.017   | Fig. S12a  |
| top-hcp        | -0.027   | 0.013    | -0.020   | Fig. S12b  |
| fcc-hcp        | 0.002    | -0.002   | -         | Fig. S12c  |
| Y-terminated YCo$_2$(111) |          |          |          |            |
| top-fcc        | 0.005    | -0.003   | 0.003    | Fig. S12d  |
| top-hcp        | 0.003    | -0.001   | -0.002   | Fig. S12e  |
| fcc-hcp        | -0.012   | 0.006    | -         | Fig. S12f  |
**Table S7:** Results obtained for gr/bulk-like-YCo$_2$(111): $\Delta E$ (in eV/C-atom) is the relative total energy with respect to the energetically most favourable structure; $d_0$ (in Å) is the mean distance between the graphene overlayer and the interface substrate layer; $d_1$ (in Å) is the mean distance between the interface substrate layer and the second substrate layer; $d_2$ (in Å) is the mean distance between the second substrate layer and the third substrate layer; $d_3$ (in Å) is the mean distance between the third substrate layer and the fourth substrate layer; $m_{\text{Co}}(\mu_B)$ is the Co spin magnetic moment (two values are given for the interface/bulk atoms); $m_{\text{Y}}(\mu_B)$ is the Y spin magnetic moment.

| Structure          | $\Delta E$ | $d_0$ | $d_1$ | $d_2$ | $d_3$ | $m_{\text{Y}}$ | $m_{\text{Co}}$ | Reference     |
|--------------------|------------|-------|-------|-------|-------|---------------|---------------|---------------|
|                    |            |       |       |       |       |               |               |               |
| Co-terminated YCo$_2$(111) |           |       |       |       |       |               |               |               |
| top-hcp            | 0.00       | 2.03  | 1.19  | 0.77  | 0.61  | $-0.155$      | 1.273/0.019   | Fig. S13a     |
| top-fcc            | 0.01       | 1.98  | 1.17  | 0.79  | 0.49  | $-0.154$      | 1.232/0.026   | Fig. S13b     |
| fcc-hcp            | 0.13       | 2.86  | 1.21  | 0.86  | 0.44  | $-0.293$      | 1.359/0.007   | Fig. S13c     |
|                    |            |       |       |       |       |               |               |               |
| Y-terminated YCo$_2$(111) |           |       |       |       |       |               |               |               |
| top-hcp            | 0.02       | 2.53  | 1.71  | 1.53  | 0.61  | $-0.260$      | 1.116/0.005   | Fig. S13d     |
| top-fcc            | 0.02       | 2.52  | 1.70  | 1.53  | 0.61  | $-0.254$      | 1.123/0.011   | Fig. S13e     |
| fcc-hcp            | 0.00       | 2.34  | 1.73  | 1.53  | 0.61  | $-0.265$      | 1.113/0.008   | Fig. S13f     |
Table S8: Interface C spin magnetic moment (several values for the nonequivalent carbon atoms are indicated) of gr/bulk-like-YCo$_2$(111).

| Structure   | $m_{C1}$ | $m_{C2}$ | $m_{C3}$ | Reference  |
|-------------|----------|----------|----------|------------|
| Co-terminated YCo$_2$(111) |          |          |          |            |
| $top$-fcc   | $-$0.015 | 0.019    | $-$0.028 | Fig. S13a  |
| $top$-hcp   | $-$0.016 | 0.014    | $-$0.031 | Fig. S13b  |
| $fcc$-hcp   | 0.001    | $-$0.003 | -        | Fig. S13c  |
| Y-terminated YCo$_2$(111) |          |          |          |            |
| $top$-fcc   | 0.007    | 0.004    | 0.002    | Fig. S13d  |
| $top$-hcp   | 0.006    | 0.002    | 0.002    | Fig. S13e  |
| $fcc$-hcp   | 0.001    | $-$0.004 | -        | Fig. S13f  |
Figure S1: Top views of the crystallographic structures of gr/Co(0001): (a) *top-fcc* – the C atoms are placed directly above the Co atoms of the first layer (*top* site) and the *fcc* hollow site; (b) *top-hcp* – the C atoms are placed directly above the Co atoms of the first layer (*top* site) and the second layer (*hcp* site); (c) *fcc-hcp* – the C atoms are *fcc* and *hcp* hollow sites. The energetically most favourable structure is surrounded by the red rectangular.
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Figure S3: Spin-resolved band structures calculated for gr/Co(0001). The weight of the C-$p_z$ and Co-$3d$ states in the band structures is proportional to the width of the colored line.
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Figure S6: Spin-resolved band structures calculated for gr/1 ML-Y/Co(0001). The weight of the C-$p_z$ and Y-$3d$ states in the band structures is proportional to the width of the colored line.
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Figure S11: (a) Density of state for paramagnetic bulk YCo$_2$. (b,c) Spin-resolved density of states obtained for the Co- as well as Y-terminated YCo$_2$(111) slabs.
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