Supplemental Materials for "**Ab initio simulations of defect-based magnetism: The case of CoSi nanowires**"

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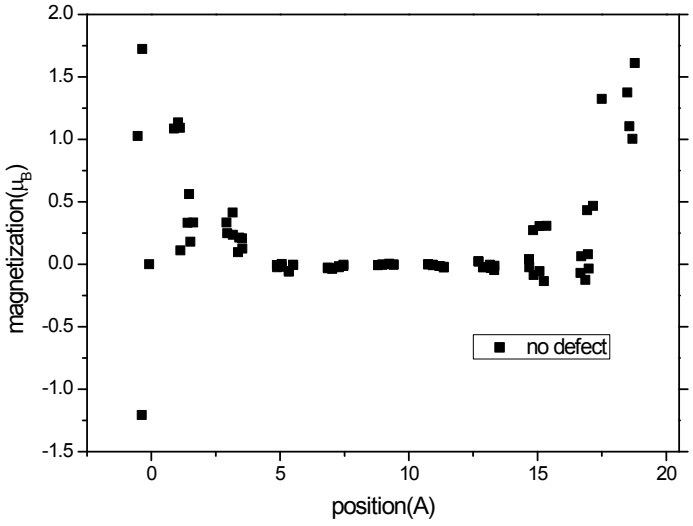


Figure S1. Distribution of simulated moment of Co atoms around SiO_2/CoSi (without ordered vacancies)/SiO_2 interface and the chosen three Co atoms with different distances to the interface based on LDA+U for single k-point and total drift force less than 0.17 eV/Å(https://www.materialsproject.org/materials/mp-18748/GGA+U, Co 3.32eV, the Ceder's Materialsproject home page)

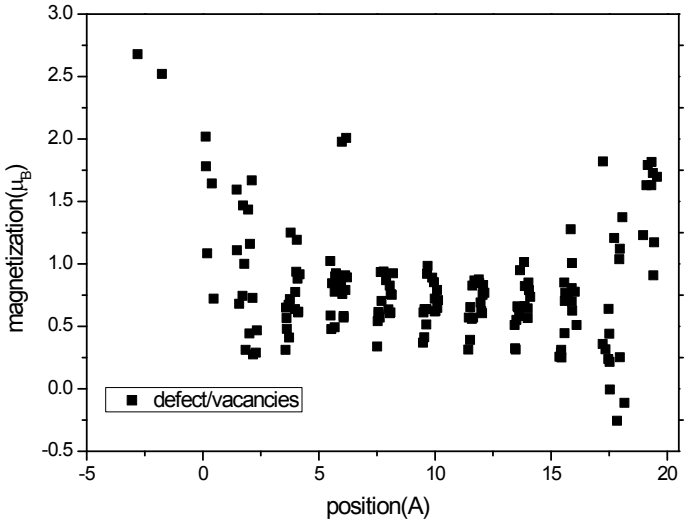
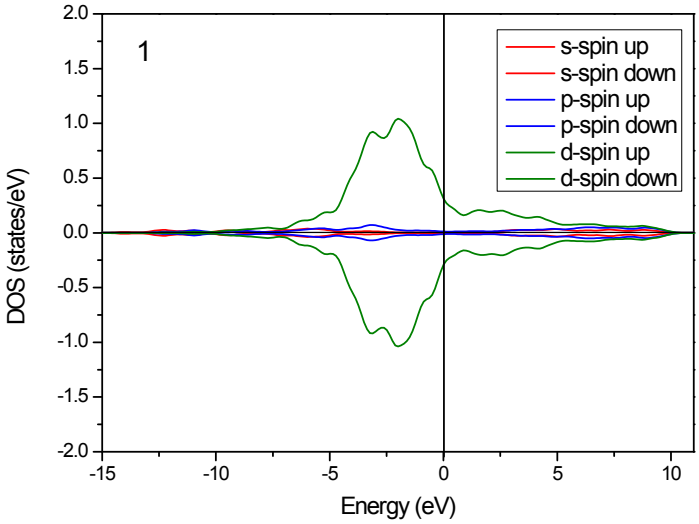
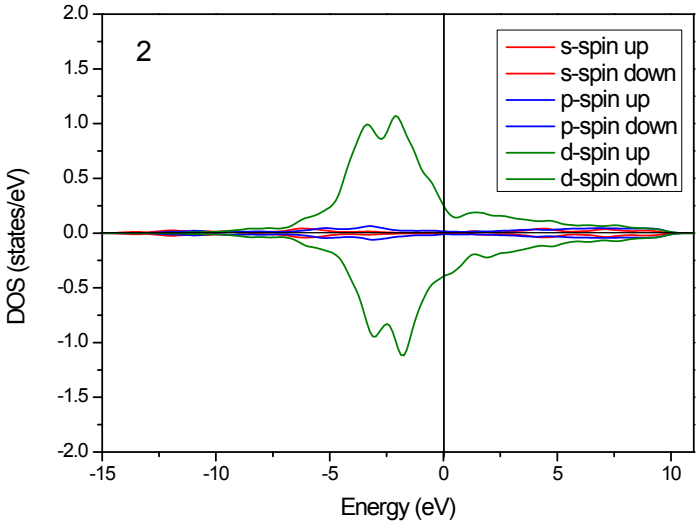


Figure S2. Distribution of simulated moment of Co atoms around SiO_2/CoSi (with ordered vacancies)/SiO_2 interface and the chosen three Co atoms with different distance to the interface based on LDA+U


1
s-spin up
s-spin down
p-spin up
p-spin down
d-spin up
d-spin down
DOS (states/eV)
Energy (eV)
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-15
-10
-5
0
5
10


2
s-spin up
s-spin down
p-spin up
p-spin down
d-spin up
d-spin down
DOS (states/eV)
Energy (eV)
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-15
-10
-5
0
5
10

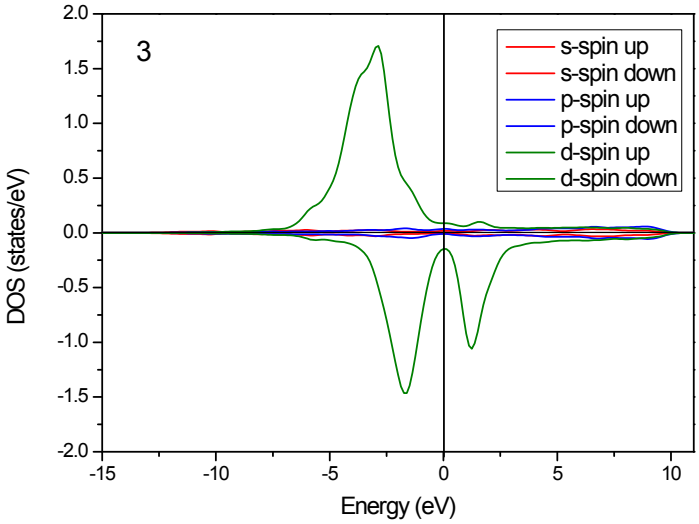
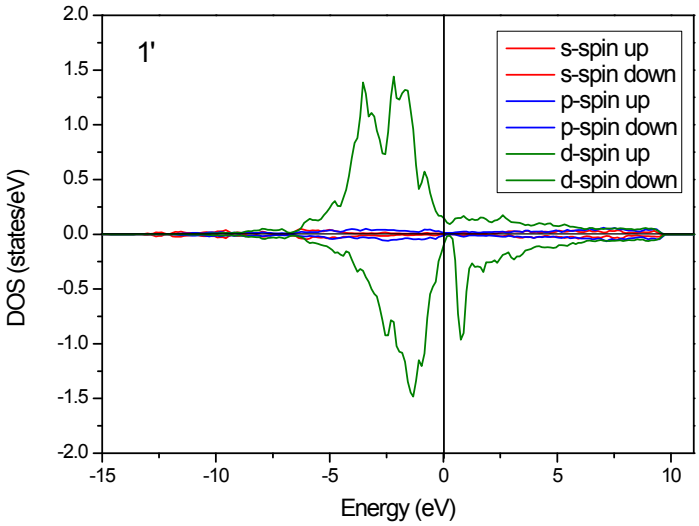


Figure S3. Corresponding DOS's of Fig.3 (LDA+U)



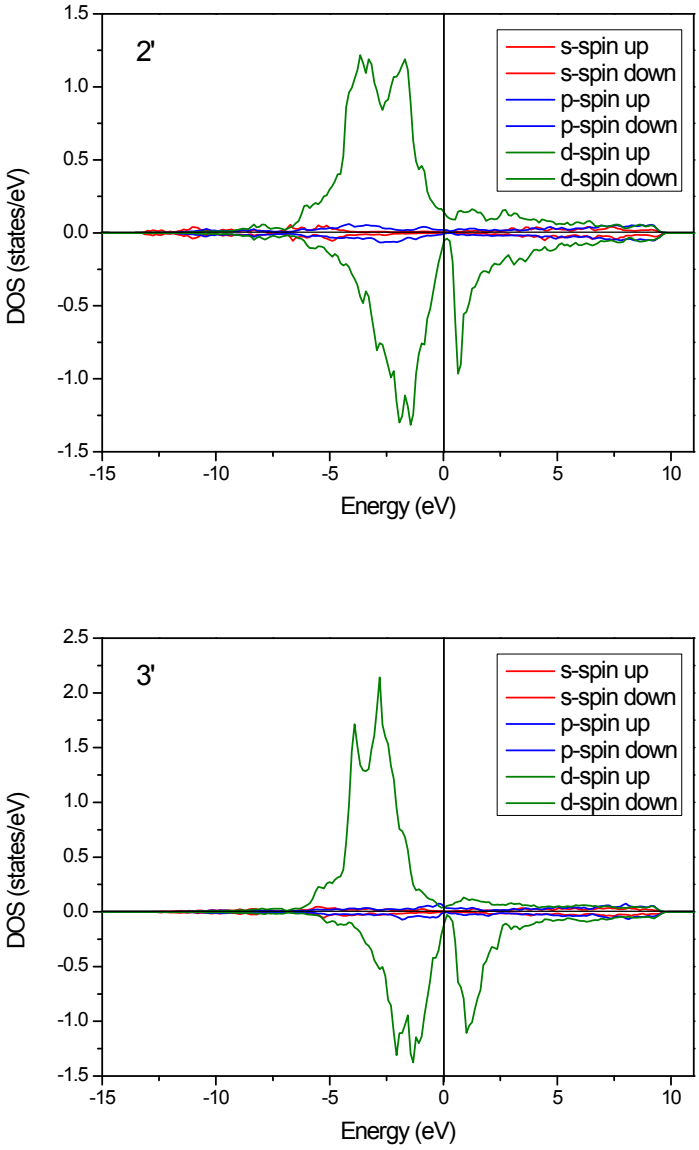


Figure S4. Corresponding DOS's of Fig. 4 (LDA+U), which become less symmetric due to existence of vacancies.

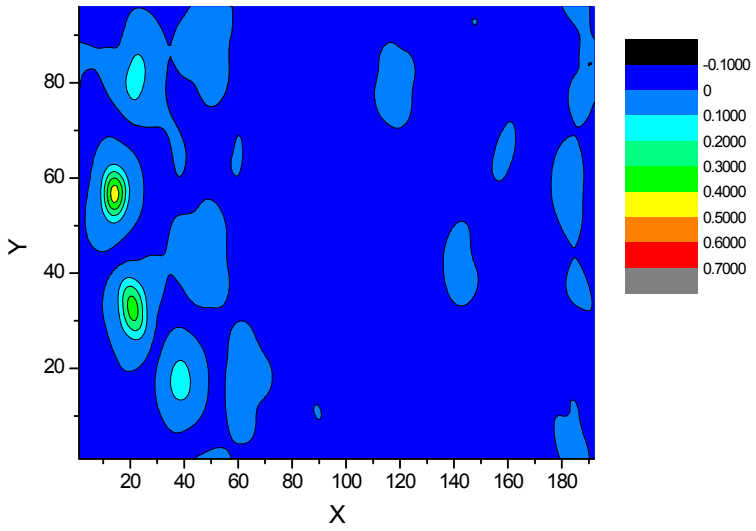


Figure S5. Contour of the electron density for spin-up minus spin-down at the 2’ atom layer. (Y along [211] in the nanowire(long axis) and X along the inward direction in Fig. 4 in unit of Å)

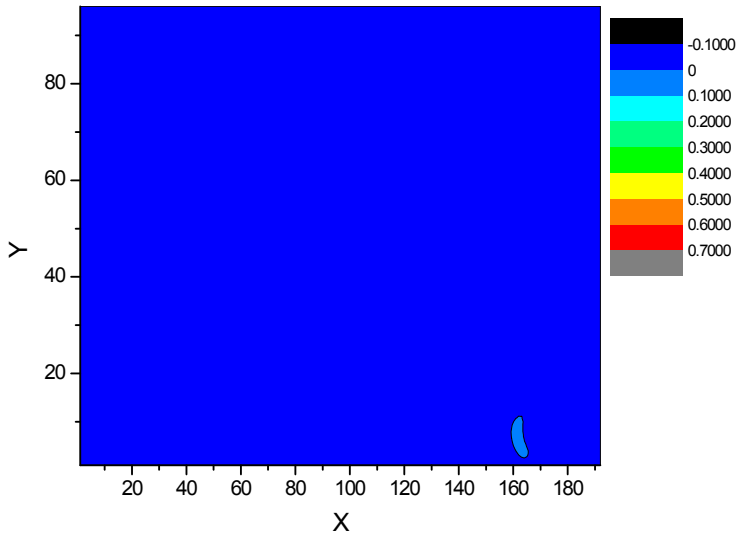


Figure S6. Contour of the electron density for spin-up minus spin-down at the 1’ atom layer(Y along [211] in the nanowire(long axis) and X along the inward direction in Fig. 4 in unit of Å)