

## Supplementary Information

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### **Field-effect transistors fabricated from diluted magnetic semiconductor colloidal nanowires**

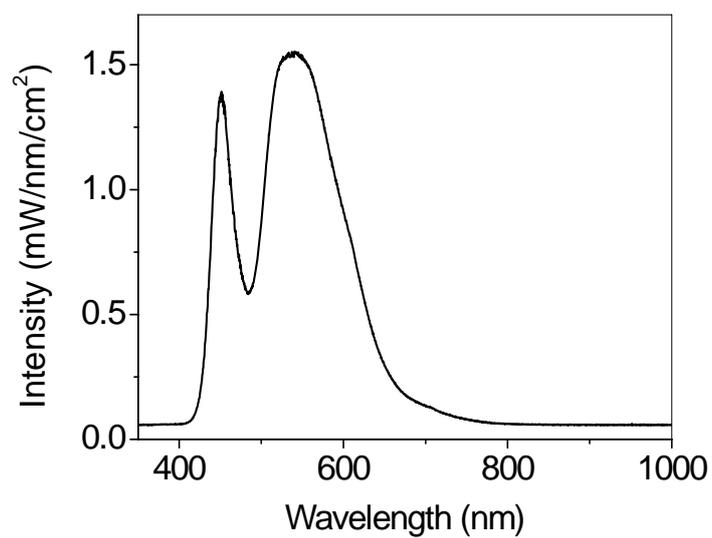
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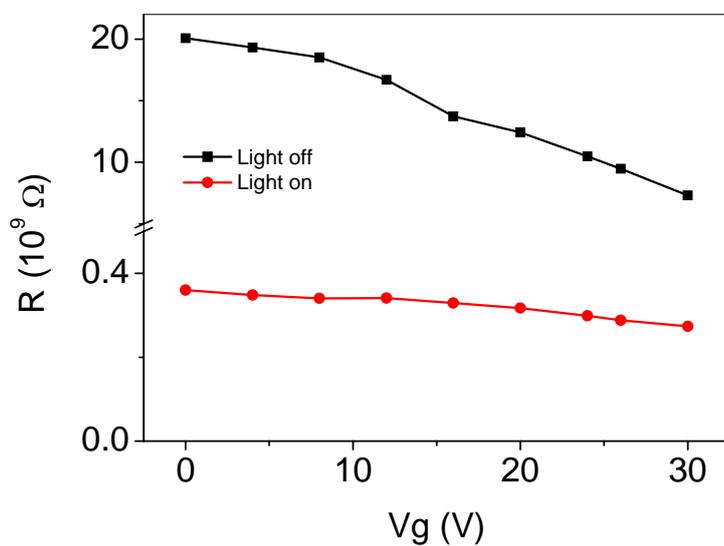
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### Theoretical calculations

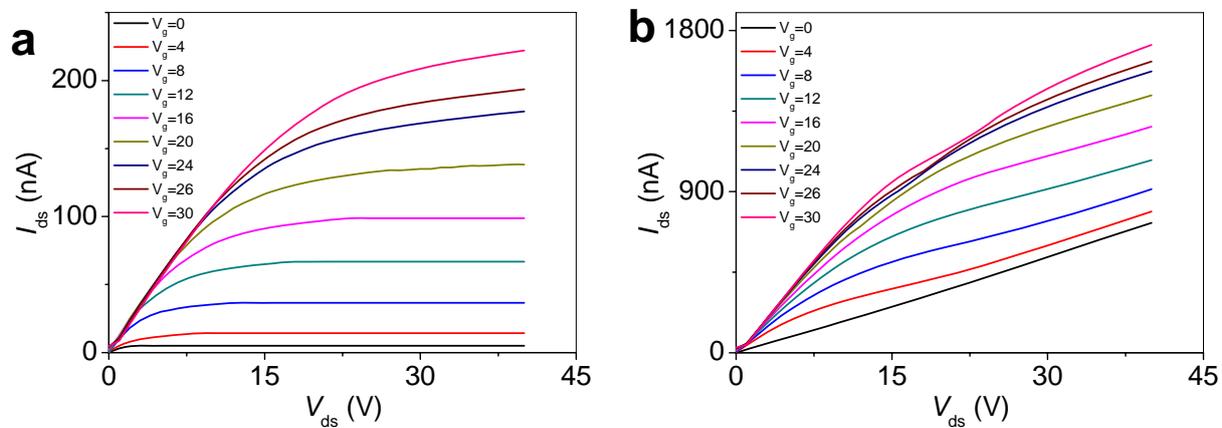
An individual CdSe nanowire was modelled as Cd<sub>54</sub>Se<sub>54</sub> geometry with a diameter of around 22 Å in a supercell (Figure S5). The electronic structures of pure and Co<sup>2+</sup>-doped CdSe nanowires were determined using spin-polarized plane-wave density functional calculations, as implemented in the Vienna *Ab-initio* Simulation Package (VASP).<sup>1, 2</sup> Projected augmented wave pseudopotential based on local density approximation<sup>3</sup> is adopted to treat the core electron.<sup>4, 5</sup> The vacuum spaces in both X and Y dimensions are 15 Å, which is enough to separate the interaction between periodic images. The cutoff energies for plane waves are chosen to be 275 eV. A Monkhorst pack mesh of 1 × 1 × 11 and 1 × 1 × 41 K-points<sup>6</sup> are used for sampling the one dimensional Brillouin zone during geometry optimization and band structure calculations, respectively. The convergence tolerance of force on each atom during structure relaxation was set at 0.006 eV/Å.



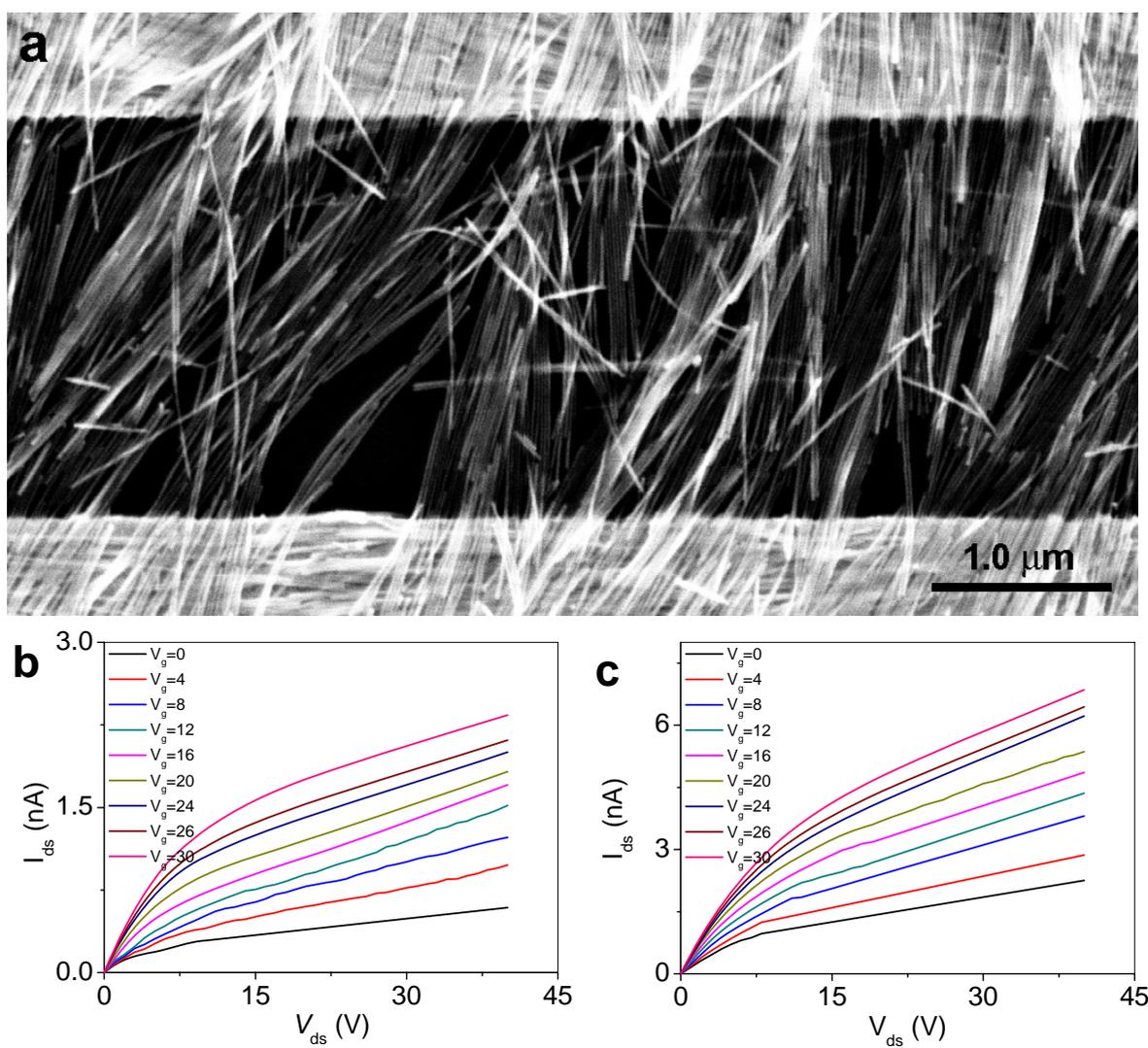
**Figure S1.** The spectrum of microscope light used for irradiation.



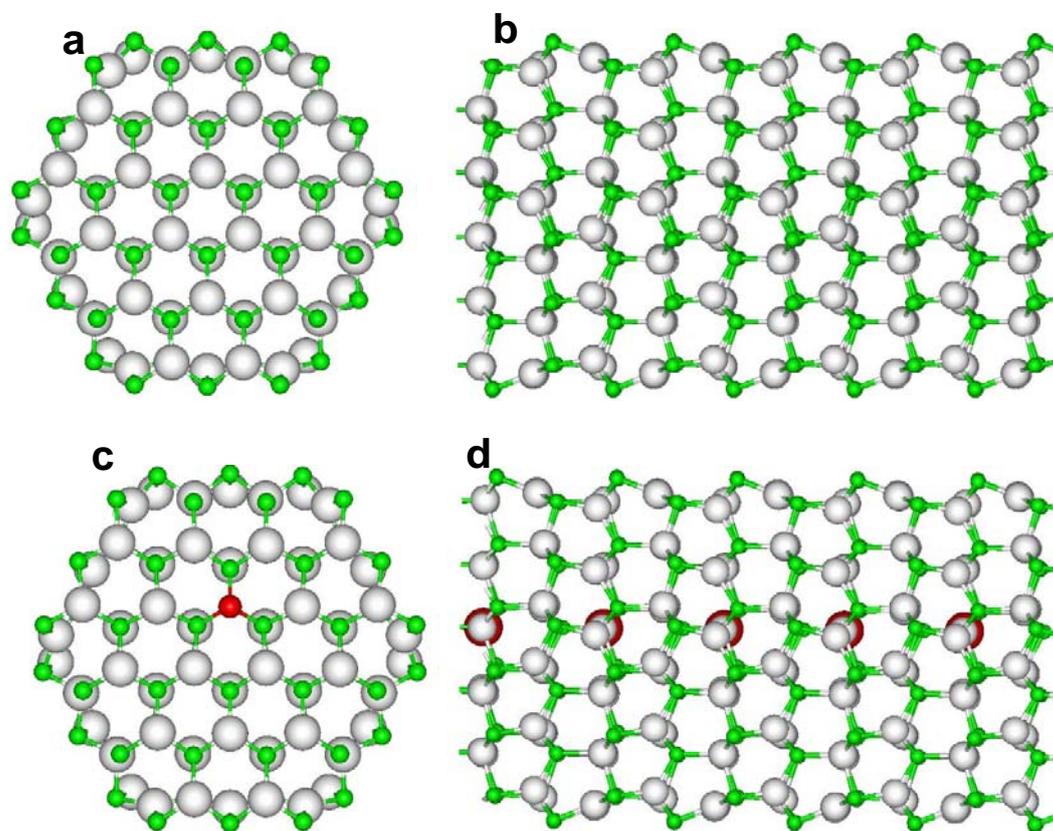
**Figure S2.** The variation of resistivity with the gate voltage applied in the presence and absence of light irradiation. The voltage between source and drain is fixed at 38 V.



**Figure S3.**  $I$ - $V$  curves of doped nanowire-based FET devices measured in the absence (a) and presence (b) of light irradiation after two weeks storage.



**Figure S4.** (a) Typical SEM image of CdSe nanowires between the source and drain electrodes of as-fabricated FET device; (b-c)  $I$ - $V$  curves of CdSe nanowire-based FET device measured in the absence and presence of light irradiation.



**Figure S5.** Computational models of undoped CdSe (**a-b**) and Co<sup>2+</sup>-doped CdSe (**c-d**) nanowire. White, green and red balls represent Cd, Se and Co atoms, respectively.

## References

1. G. Kresse and J. Furthmuller, *Phys. Rev. B*, 1996, **54**, 11169.
2. G. Kresse and J. Furthmuller, *Comput. Mater. Sci.*, 1996, **6**, 15.
3. D. M. Ceperley and B. J. Alder, *Phys. Rev. Lett.*, 1980, **45**, 566.
4. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865.
5. P. E. Blochl, *Physical Review B*, 1994, **50**, 17953.
6. H. J. Monkhorst and J. D. Pack, *Physical Review B*, 1976, **13**, 5188.
7. R. Stranger, L. Dubicki and E. Krausz, *Inorg. Chem.*, 1996, **35**, 4218.