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Quantum Confinement and Non-Magnetic-Doped Dilute Magnetic Semiconductors[1] HYUNWOOK KWAK, University of Minnesota, TZU-LIANG CHAN, JAMES R. CHELIKOWSKY, University of Texas — Dilute magnetic semiconductors are of interest for their unique magnetic properties and their promising role in development of "spintronic" semiconductor devices. Recently, a new dimension has been brought to this class of material by observing room temperature ferromagnetism in non-magnetic doped semiconductors and insulators. Using real-space pseudopotential applied to nitrogen-doped ZnO nanowires and nanocrystals, we report the theoretical evidence of magnetism in spatially confined non-magnetic doped semiconductor nanocrystals. Detailed electronic structures and magnetic properties are examined by comparing the total energy of different spin orderings and defect configurations. Besides the prediction of high Curie temperature, our results show that the ferromagnetic order becomes more stable when the nitrogen defects experience strong quantum confinement.

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