



School of Nano Science



IPM Condensed Matter &  
Statistical Physics Group

## Weekly Seminar

### Coherence of Coupled Dangling-Bond Pairs on a Silicon Surface

Invited Speaker:

**Dr. Zahra Shaterzadeh Yazdi**

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#### **Abstract:**

Dangling bonds on semiconductor surfaces are known as truly atomic-scale quantum dots. In recent years, experiments have shown that dangling bonds located close enough to each other display coupling behavior. In this presentation, we characterize coherence and coupling strength of dangling-bond pairs that are sharing an excess electron and are located on the phosphorous-doped hydrogen-terminated silicon(100)-2x1 surface. We employ ab-initio time-dependent density functional theory technique to investigate the tunneling rate for various dangling-bond pair configurations. The results show that the coupling strength depends strongly on the structure of silicon surface and the location and orientation of dangling-bonds orbitals. Furthermore, location of the doped phosphorous with respect to both dangling bonds has a significant effect on the coherence of the excess-electron tunneling as well as the strength of dangling bonds coupling. Coupled dangling bonds can be employed as the building block for designing planar nanoscale circuits and nanostructures such as dangling-bond nanowires, quantum-cellular-automata cells, and quantum computing schemes. Therefore, learning about bonding strength and coherence of different dangling-bond pair configurations provides a better understanding of the effect of the surface structure on the construction of such systems.

Wednesday, 20<sup>th</sup> of Bahman(1395) (February 8<sup>th</sup>, 2017), 14:00-15:00

Farmaniyeh seminar room