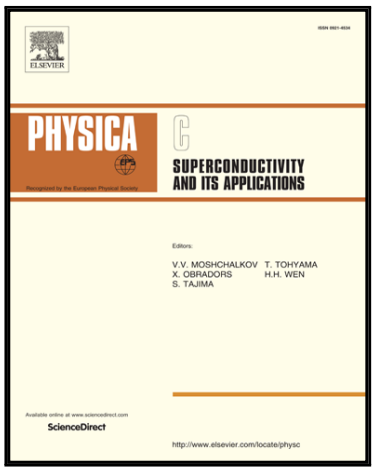

Magnetic behavior of Si-Ge bond in Si_xGe_{4-x} nano-clusters

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Highlight

- It was found that the silicon atom generally makes a stronger bond with CO than germanium and thereby preferentially affects the shape of structures having higher multiplicity. In Si-Ge structures with higher spin more than 95 % of spins accumulate on positions with less bonds to other atoms of the cluster. Through CO adsorption on these clusters bridge structures are made that behave as spin bridge which conduct the spin from the nano-cluster surface to the adsorbate atoms. A better understanding of bridged structures was achieved upon introducing the 'spin bridge' concept. Based on exhaustive spin density analysis, it was found that the reason for the extra negative charge on oxygen in the bridged structures is the relocation of spin from the surface through the bridge.