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## Electronic and magnetic properties of one and two dimensional monolayer $MoS_2$ with sulfur line defect

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Stimulated by the recent experimental observation that the single sulfur vacancies in monolayer $MoS_2$ are mobile under the electron beam and easily agglomerate into the sulfur line defects the electronic and magnetic properties of one and two dimensional (1D and 2D) monolayer $MoS_2$ with one or two staggered sulfur line defects (SV or DV), parallel to their armchair (AC) or zigzag (ZZ) direction, denoted as AC-SV, AC-DV, or ZZ-SV, ZZ-DV, respectively, have been investigated systematically by the first-principles calculations. It is found that: 1) The 2D monolayer embedded by the AC-SV or AC-DV types of sulfur line defects are all insulators with band gap values much smaller than that of a perfect monolayer. 2) More interestingly, the out-of plane deformation in 2D monolayer $MoS_2$ with ZZ-SV or ZZ-DV types of sulfur line defects can further decrease the gap value seriously or even make the band gap nearly closed. 3) Additionally, the 1D armchair $MoS_2$ nanoribbons with SV or DV types of sulfur line defects are both nonmagnetic semi-conductors. However, the defective zigzag ones are both metal with ferromagnetic coupling along the same edge, similar to that of pristine ones. 4) Finally, the stability calculations indicate that the AC-SV type of sulfur line defect in 2D monolayer $MoS_2$ is the most stable one, predicting its possible realization in the future experiments of the monolayer $MoS_2$ growth. Our simulation results can provide a new sight for engineering the electronic structures of $MoS_2$-based materials.

### Biography

Yang Han is a PhD candidate in the Department of Physics, Nanjing University in China, under the supervision of Prof. Jinming Dong. Her current researches focus on the confined growth and physical properties of the low-dimensional nanomaterials by both the molecular dynamics simulations and first principles calculations. She has published 6 papers in reputed journals, one of which has been selected to be highlighted by editorial office of the journal of Nanotechnology.

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## Comparative codeposition of Ni-Zn in acid solutions

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The reaction kinetic of Zn-Ni codéposition was investigated in acid solutions. The effects of solution composition and pH were analyzed. Results obtained in the work show that it is possible to obtain alloys rich in either nickel or zinc, from an acidic solution, depending on the Ni/Zn concentration ration. For Ni/Zn concentration ratios in the range of 1-5, zinc rich alloys are obtained despite Zn is the less noble metal and even when it is present in lower concentration than nickel. For the highest Ni/Zn concentrations ratio ≥100, the formation of the alloy occurs by a normal deposition, resulting in Ni-rich alloys. Boric acid extends the proton discharge potential to more cathodic values. Thus it can reduce anomalous codeposition since the presence of 0,8M of acid reduces the intensity of the peak corresponding to δ phase that is rich in zinc and enhances the intensity of γ phase containing more nickel than the δ phase.

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