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Formation of metallic gold chain on patterned hydrogen terminated Si(001)-2×1 surface: Density functional study BIKASH GUPTA, PURUSOTTAM JENA, Department of Physics, Virginia Commonwealth University, Richmond, VA 23284 — Metal adsorption on silicon surface for the formation of linear metallic chain is one of the important research areas for the advancement of nanotechnology. Due to the presence of dangling bonds all over the surface of bare Si(001), metals when deposited, generally do not tend to form stable wire structures. However, patterned hydrogen terminated Si-surface may be a good choice for the formation of atomic chain structures of metals. Since patterned hydrogen terminated Si(001):2x1 surface is very stable, we consider patterning it by removing desired hydrogen atoms and adsorbing gold atoms. We have examined the structure, energetic and electrical properties of such gold adsorbed surface by varying gold coverage. We have found that linear gold chain structures may be formed by controlling gold coverage. Some of these gold chain structures are metallic in nature. We hope that our results will motivate synthesis of gold chains on patterned hydrogen terminated Si(001): 2×1 surface.

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