Abstract Submitted
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Computational study of hydrogen adsorption on silica-based nanosprings YINGQIAN ZHAN, MARTY YTREBERG[1], Univ. of Idaho — Silica-based nanosprings were recently synthesized and characterized by McIlroy and collaborators.1 Further experimental studies on these nanosprings revealed a high adsorption rate of hydrogen gas at room temperature (data not published). In this study, computer simulation was used to understand the hydrogen adsorption properties of silica nanosprings. The interaction between the nanomaterial and hydrogen molecules was described using classical approximations. Different orientations and positions of the hydrogen molecule relative to the nanosprings were tested and the effect of the separation between the two nanowires was studied. The results suggest that the hydrogen molecule tends to be trapped between the nanosprings, i.e., that the unique geometry of the nanosprings is the cause for the high rate of adsorption. References 1.Lidong Wang, D Major, P Paga, D Zhang, M G Norton and D N McIlroy. Nanotechnology, 2006, 17, S298-S303

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