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The effect of the sodium and iodine doping on the electronic band structure of the polyicosahedral Si nanowire: A first principles study. KENGO NISHIO, Research Institute for Computational Sciences (RICS), National Institute of Advanced Industrial Science & Technology (AIST), TAISUKE OZAKI, TETSUYA MORISHITA, WATARU SHINODA, MASUHIRO MIKAMI, JAIST — In a previous molecular dynamics study, we predicted a polyicosahedral Si nanowire which has a Si20 fullerene cage per icosahedral Si100 nanodot [1]. The unique cage structure is distinct from the crystalline diamond Si nanowire. Encapsulating a guest atom into the Si20 cage allows us to tune the physical properties of the nanowire. Here, we report on a first-principles study of the effect of the sodium and iodine doping on the electronic band structure of the hydrogen-terminated polyicosahedral Si nanowire [2]. Our calculations reveal that the guest-free polyicosahedral Si nanowire is a semiconductor with a 1.20 eV band gap. We also find that the semiconducting nanowire becomes metallic by the sodium and iodine doping, suggesting that the electronic band structure of polyicosahedral Si nanowires can be tuned by doping appropriate guest atoms. [1] J. Chem. Phys. 125, 074712 (2006). [2] submitted to PRB

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