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Structural, Electronic and Vibrational Properties of Na_xSi_{136} ($0 < x < 24$) Clathrates CRAIG HIGGINS, EMMANUEL NENGHABI, CHARLES MYLES, Texas Tech University, KOUSHIK BISWAS, Oak Ridge National Laboratory, MATT BEEKMAN, University of Oregon, GEORGE NOLAS, University of South Florida — CRAIG HIGGINS, EMMANUEL NENGHABI[†], CHARLES W. MYLES, Texas Tech U.; KOUSHIK BISWAS, Oak Ridge National Lab; MATT BEEKMAN, U. of Oregon; GEORGE S. NOLAS, U. of South Florida - Na_xSi_{136} is a Type II clathrate with important thermoelectric properties. It's face-centered cubic lattice contains polyhedral "cages" of silicon atoms with Na atom "guests" in the cages. This material is very interesting because powder X-ray diffraction experiments[1]for differing Na content x have shown that, for increasing x in the range $0 < x < 8$, lattice contraction occurs. After all Si_{28} cages in the unit cell are filled ($x = 8$) and x is increased further, causing a filling of the Si_{20} cages, a contrasting lattice expansion results. Using the local density approximation, we have calculated the x dependences of the structural, electronic and vibrational properties of Na_xSi_{136}. Results are presented for the x dependences of the lattice constant, electronic bands, and vibrational modes. Our results for the x dependence of the lattice constant are in agreement with our X-ray data[1]. [†]Deceased. [1]M. Beekman, E.N. Nenghabi, K. Biswas, C.W. Myles, M. Baitinger, Y. Grin, G.S. Nolas, Inorg. Chem. 49, 5338–5340 (2010).

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