

Abstract Submitted
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Tetra, a modeling system for the generation of the atomic configurations of branched wurtzite/zincblende nanostructures¹ PETER GRAF, KWISEON KIM, WESLEY JONES, National Renewable Energy Laboratory, LINWANG WANG, Lawrence Berkeley National Laboratory — The first step in simulating properties of nanostructures is generation of accurate atomic configurations. For complex objects such as the multiply branched heterostructures synthesized by Alivisatos et al.¹, this is nontrivial. We report here on our code, “tetra,” that accomplishes this task. Borrowing from techniques of computer graphics, we represent the complex structure as a tree, each node of which is a shape with fixed crystal structure, and use concatenation of 4 by 4 homogeneous transformation matrices to arrange these fixed building blocks into the final object. A simple text based input “language” describes the connectivity and dimensions of the structure. The ultimate purpose of this code is use within a package that will explore and optimize electronic properties of such structures with respect to their geometry². We will present examples of both structures and subsequent semi-empirical pseudopotential-based³ electronic structure calculations. [1] A. P. Alivisatos, et al., *Nature*, **430**, 190 (2004). [2] J. Li and L. W. Wang, *NanoLetters*, **3**, 10, 1357-1363 (2003). [3] L. W. Wang and A. Zunger, *Phys. Rev. B* **51**, 17398 (1995).

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