

## Documents

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**B-Splines and NURBS based finite element methods for strained electronic structure calculations**

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**Abstract**

This paper presents B-splines and nonuniform rational B-splines (NURBS)-based finite element method for self-consistent solution of the Schrödinger wave equation (SWE). The new equilibrium position of the atoms is determined as a function of evolving stretching of the underlying primitive lattice vectors and it gets reflected via the evolving effective potential that is employed in the SWE. The nonlinear SWE is solved in a self-consistent fashion (SCF) wherein a Poisson problem that models the Hartree and local potentials is solved as a function of the electron charge density. The complex-valued generalized eigenvalue problem arising from SWE yields evolving band gaps that result in changing electronic properties of the semiconductor materials. The method is applied to indium, silicon, and germanium that are commonly used semiconductor materials. It is then applied to the material system comprised of silicon layer on silicon-germanium buffer to show the range of application of the method. © 2018 by ASME.

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