# Using Isogeometric Analysis in Electronic Structure Calculations

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## ABSTRACT

In electronic structure calculations, various material properties can be obtained by means of computing the derivatives of the total energy w.r.t. atomic positions. The derivatives, also known as Hellman-Feynman forces, require, because of practical computational reasons, the discretized charge density and wave functions having continuous second derivatives in the whole solution domain. We describe an application of isogeometric analysis (IGA) [2], a spline modification of finite element method (FEM) [4], to achieve the required continuity. The technique of Bezier extraction [1] is used for adding the IGA capabilities to our FEM based code [6] for ab-initio calculations of electronic states within the density-functional framework [3, 5], based on the open source finite element package SfePy (http://sfepy.org). We compare FEM and IGA convergence properties and present several numerical results. The work was supported by the Grant Agency of the Czech Republic, project P108/11/0853 and the grant project of the Czech Science Foundation (GACR), No. GAP 101/12/2315, within the institutional support RVO:61388998.

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