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Study of the Mott-insulator TiOCl under pressure and doping YUZHONG ZHANG, ROSER VALENTI, HARALD JESCHKE, Johann Wolfgang Goethe-Universität, Institut für Theoretische Physik, S. GLAWION, M. SCHLACHTER, K. GOß, M. SCHOLZ, M. SING, R. CLAESSEN, Experimentelle Physik 4, Am Hubland, University of Würzburg, D-97074 Würzburg, Germany — We will discuss recent experiments of the Mott-insulator TiOCl under pressure and Na doping in the frame of Density Functional Theory (DFT) calculations where we employ Car-Parrinello molecular dynamics with Projected Augmented Wave (PAW) wavefunctions. For TiOCl under pressure a phase transition from insulator to metal is found as observed experimentally. For the doped system we have considered supercells of Na doped TiOCl and we propose possible effective models for the mechanism of doping.

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