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Insulator – polaron conductor – metal transitions in a complex oxide $12CaO{\cdot}7Al_2O_3$. P. SUSHKO, A. SHLUGER, A. STONEHAM, Department of Physics and Astronomy, University College London, UK, K. HAYASHI, S. MATSUISHI, M. HIRANO, H. HOSONO, Frontier Collaborative Research Center, P.O. Box S2-13, Tokyo Institute of Technology, Japan — Recent experiments have demonstrated that a complex nano-porous oxide $12CaO{\cdot}7Al_2O_3$ (C12A7) built of positively charged sub-nanometer cages can be converted from a transparent insulator to a transparent conductor by H_2 doping followed by UV-light irradiation with 4–4.5 eV photons [1]. This irradiation induces optical absorption bands with maxima at 0.4 eV and 2.8 eV and high concentrations of unpaired electrons. We use ab initio calculations to reveal the mechanism of photo-induced insulator–conductor transition and the role of H atoms in this process and to elucidate the transport properties of the electrons in this system as a function of electron concentration. Our theoretical modeling suggests that at concentration below 10^{20} cm^{-3} electrons are responsible for the polaron type electrical conductivity with the activation energy close to 0.1 eV as well as for the optical absorption at 0.4 eV and 2.8 eV [2]. We demonstrate that, as the electron concentration exceeds 10^{20} cm^{-3}, the character of electronic conductivity changes from polaron type to metallic. [1] K. Hayashi et al., Nature **419**, 462 (2002). [2] P.V. Sushko, et al., Phys. Rev. Lett. **91**, 126401 (2003); P.V. Sushko et al., Appl. Phys. Lett. **86**, 092101 (2005).

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