Insulator – polaron conductor – metal transitions in a complex oxide 12CaO·7Al2O3. 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·7Al2O3 (C12A7) built of positively charged sub-nanometer cages can be converted from a transparent insulator to a transparent conductor by H2 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).