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First-Principles Study of Er Location in Er-Si Systems with Oxygen Co-Dopants R.H. PINK, JUNHO JEONG, DIP N. MAHATO, M.B. HUANG, T.P. DAS[1], SUNY Albany, R.H. SCHEICHER, MTU Houghton, SITARAM BYAHUT, Tribhuvan University, Kathmandu, Nepal — Using the Hartree-Fock cluster procedure, we are investigating possible models for the Er^{3+} ion in silicon with oxygen co-dopants[1]. We are examining first the Hi (hexagonal interstitial) site with six O atoms in the intrabond regions of the six Si-Si bonds for this center[2], allowing for relaxation in positions of the O and Si atoms. The aim of this study is to see if the presence of the O atoms is indeed able to change the situation of a maximum in the potential surface for Er^{3+} found from our recent investigations of the Er-Si system without co-dopants to a minimum in the co-doped Oxygen system. Results for the Er^{3+} potential curve for the Hi center and the geometries of the Si and O atoms will be presented. [1] F. d'Acapito, S. Mobilio, S. Scalese, A. Terrasi, G. Franzó and F. Priolo, Phys. Rev. B 69, 153310 (2004) and references therein. [2] J.D. Carey, J. Phys. Condens. Matter 14, 8537 (2002)

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