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Electrical properties of the α-pyrochlore $\mathbf{Bi_{2-y}Sr_yIr_2O_7}$ solid solution PABLO DE LA MORA, Facultad de Ciencias, CARLOS COSIO CASTAÑEDA, Facultad de Quimica, FRANCISCO MORALES LEAL, Instituto de Investigacion en Materiales, GUSTAVO TAVIZON, Facultad de Quimica, Universidad Nacional Autonoma de Mexico — To study the electrical properties of the $Bi_{2-y}Sr_yIr_2O_7$ ($\{Ir_2O1_6\}\{Bi_{2-y}Sr_yO2\}$) solid solution *ab-initio DFT* (*WIEN2k*) calculations were done. In this compound, when Sr is introduced the resistivity increases and the ρ/T slope also increases. In this system the $Bi_{2-y}Sr_yO2$ substructure has little contribution to the conductivity, even so, it is indirectly responsible to the conductivity modifications, since it affects the other substructure; Ir_2O1_6, which is conducting. When Bi is substituted by Sr, it pushes $O1$, shortening the Ir-$O1$ bond and the resistivity is supposed to decrease; instead a small increment is found. What is found is that this increment is due to the relaxation time, τ. There are two contributions to τ; a) static; the random replacement of Bi by Sr introduces 'impurities', shortening τ, therefore increasing the resistivity, b) dynamic; due to the thermal oscillations of the atoms. What is found is that the effect of the oscillations in the compound with Sr has a larger impact on the electronic structure, thus increasing the ρ/T slope.

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