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Electronic structure and linear response properties of the crystal KIO_3: A first-principle density-functional theory study YIMING MI, XINXIN ZHAO, School of Fundamental Studies, Shanghai University of Engineering Science, China, SHUICHI IWATA, Graduate School of Frontier Sciences, The University of Tokyo, Japan — The electronic band structure and both the partial and total density of states of the ABO_3 type crystal KIO_3 are investigated based on the first principles pseudopotential plane wave approach within density functional theory formalism. The structural optimization was performed in terms of generalized gradient approximation. And the optical properties and the imaginary parts of the frequency-dependent dielectric function of the material are also calculated. The acquired calculational results of the material are in good agreement with available experimental data.

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