Hybrid density functional theory calculations for the electronic and optical properties of Fe^{3+}- doped KDP crystals

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The Fe^{3+} ion is the most common impurity ion in potassium dihydrogen phosphate (KDP) and can combine with hydrogen vacancies to form cluster defects, which can lead to optical damage of the KDP crystal. In this study, the effect of the $Fe_K^{2+} + 2V_H^-$ cluster on the crystal structure, electronic, and optical properties of KDP crystals were investigated using hybrid density functional theory, and the mechanism of Fe^{3+} ions lowering the laser-induced damage threshold of the KDP crystal was analyzed. The damage from the $Fe_K^{2+} + 2V_H^-$ cluster defect to the crystal structure of the KDP crystal was found to be greater than that from hydrogen vacancies due to the large lattice relaxation introduced by Fe_K^{2+} defects. The Fe_K^{2+} defect introduces two defect states (at 2.4 eV and 6.6 eV) into the bandgap of the KDP crystal as well as absorption peaks at around 278 nm in the xy plane. When $Fe_K^{2+} + 2V_H^-$ cluster defects form, hydrogen vacancies induce an increase in charge density around the O atoms bonded to Fe_K^{2+}, which slightly alters the interaction of the electronic states of the Fe_K^{2+} and O atoms. These cluster defects have an influence on the electronic and optical properties via charge transfer in the xy plane in the KDP crystal. This work provides a good suggestion to improve the laser-induced damage threshold of KDP crystals by decreasing the concentration of cluster defects in KDP crystals [1].

References

[1] Li Y, Liu BA, Li YL, et al. Hybrid density functional theory calculations for the electronic and optical properties of Fe^{3+}- doped KDP crystals. CrystEngComm. 2022;24:8082–8088.