First-principles study of charge states of point defects in Ti:sapphire co-doped with nonisovalent atoms
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Ti ions in titanium-doped sapphire may exist in different charge states and demonstrate a tendency to form pairs, triples and larger defect clusters \cite{1,2}. The laser efficiency of Ti:sapphire is affected by a residual infrared absorption in the emission band of the Ti:Al\textsubscript{2}O\textsubscript{3} laser. The residual absorption is caused by Ti\textsuperscript{3+}-Ti\textsuperscript{4+} pairs. In this connection, the reduction of the ratio of the concentration of isolated Ti\textsuperscript{3+} defects to the concentration of Ti\textsuperscript{3+}-Ti\textsuperscript{4+} pairs is a challenge problem.

We analyze the role of co-doping in a control of the charge state of Ti in Ti:sapphire and an influence of co-doping on the formation of Ti–Ti pairs. We consider co-doping with carbon, nitrogen and fluorine. The analysis is based on the density function theory approach implemented in the open-source DFT-package SIESTA \cite{3}.

It is found that carbon defects have high formation energy and do not affect the charge state of Ti defects. In view of low formation energy of substitutional N\textsubscript{O} defects, co-doping with nitrogen yields negative effect: the concentration of Ti\textsuperscript{3+}-Ti\textsuperscript{4+} pairs increases. In contrast, co-doping with fluorine atoms that form F\textsubscript{O}\textsuperscript{+} defects may result in an essential decrease of the concentration of Ti\textsuperscript{3+}-Ti\textsuperscript{4+} pairs. We determine the conditions at which a large ratio of Ti\textsuperscript{3+} to Ti\textsuperscript{3+}-Ti\textsuperscript{4+} can be achieved.

The band structure of Ti:sapphire co-doped with fluorine is calculated. It is established that co-doping with fluorine does not result in an appearance of additional impurity levels in the band gap, and, therefore, fluorine admixtures do not influence optical properties of Ti:sapphire.