Adsorption of gas molecules (CO, CO , NO, NO , and CH) on undoped and Ag-doped bismuth ferrite oxide (BFO) by DFT investigation

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Aims and scope

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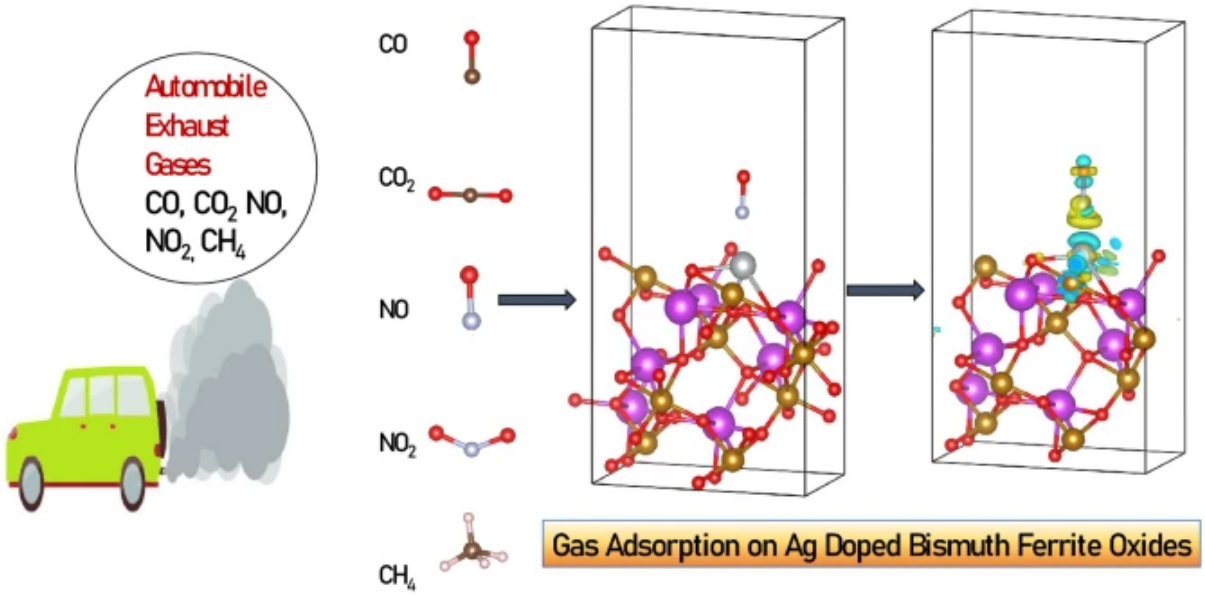
Abstract

Bismuth ferrite oxide (BFO) has enormous potential in nanoelectronics. BFO is a potential structure for the detection of hazardous gas analytes. Investigation into the adsorption of gas molecules (CO, CO_2, NO, NO_2, and CH_4) on undoped and Ag-doped BFO by density-functional theory (DFT) has been reported in the present communication. The bandgaps, density of states, total adsorption energy, charge transfer, and charge density difference are calculated for undoped and Ag-doped BFO. Band structure calculations confirm that Ag-BFO is a semiconductor with a bandgap about the fermi level. The adsorption mechanism of Ag-BFO was found to be more favourable in energy terms than pure BFO. Ag-BFO provides robust adsorption arrangements for gas molecules. During adsorption, the charge density difference accumulated over the gas molecules, indicating acceptor behaviour in reaction with Ag-BFO. This study clearly confirms that Ag-BFO can provide the most stable adsorption configurations for the adsorbed gas molecules.

Graphic abstract



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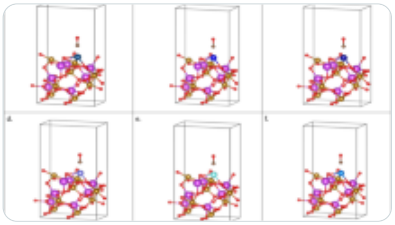

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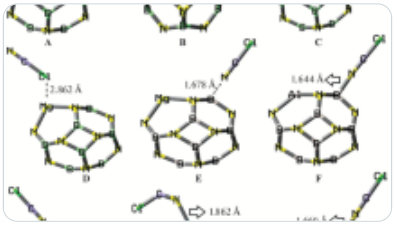

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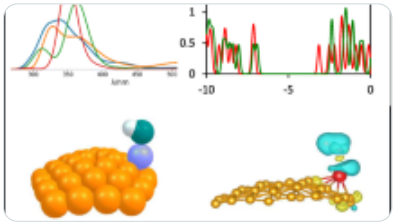

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Data availability

The data supporting this study's findings are available from Google Cloud. Still, restrictions apply to the availability of these data, which were used under licence for the current study and are not publicly available. Data are, however, available from the authors upon reasonable request and with permission of Google Cloud Console.

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Ethics declarations

Conflict of interest

The authors did not receive support from any organization for the submitted work.

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