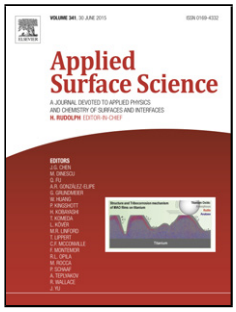

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The Effect of Oxygen Molecule Adsorption on Lead Iodide Perovskite Surface by First-Principles Calculation

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Graphical abstract

Table of Contents Image

The flat bands appearing in adsorbed system hinders the electron transfer from perovskite to electron extract layer.