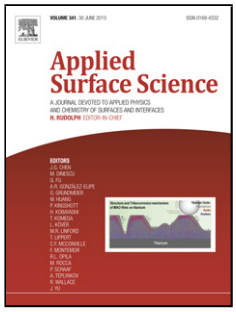

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First-principles investigation of Sn9Zn (0 0 0 1)/α-Al_2O_3 (0 0 0 1) interfacial adhesion

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Highlights

- Sn9Zn (0 0 0 1)/α-Al_2O_3 (0 0 0 1) interfacial adhesion was studied by First-principles.
- 2. O-terminated interface is favorable than that of Al-terminated.
- 3. Vacancy decreases the surface free energy.