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# First-principles investigation of Sn9Zn (0 0 0 1)/ $\alpha$ -Al<sub>2</sub>O<sub>3</sub> (0 0 0 1) interfacial adhesion

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## Highlights

- Sn9Zn (0 0 0 1)/ $\alpha$ -Al<sub>2</sub>O<sub>3</sub> (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.

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