First-principles studies of Schottky barriers and tunneling properties at Al(111)/Si(111) and $CoSi_2$(111)/Si(111) interfaces

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There has been recent interest in using Al(111)/Si(111) and $CoSi_2$(111)/Si(111) interfaces in novel merged-element transmons, which are proposed successors to the standard transmon qubits used in superconducting quantum computing [1]. We present comprehensive first-principles studies of these interfaces, studying the relaxations of the atoms near the interface, calculating the formation energies and Schottky barrier heights, and providing estimates of the Josephson critical currents based on the Simmons/Tsu-Esaki tunneling model [2,3]. We find that the formation energies and Schottky barrier heights are very similar for all Al(111)/Si(111) structures, yet vary significantly for the $CoSi_2$(111)/Si(111) structures. We attribute this to the more covalent character of bonding at $CoSi_2$/Si, which leads to configurations with distinct atomic and electronic structure. Our estimated Josephson critical currents, which govern the behavior of merged-element transmons, provide insight into the trends as a function of Schottky barrier height. We show that desirable qubit frequencies of 4–5 GHz can be obtained with a Si barrier thickness of 5–10 nm, and demonstrate that the critical current density as a function of Schottky barrier height can be modeled based on the tunneling probability for a rectangular barrier. We compare with experimental results where available, and discuss the implications of our results for actual devices.

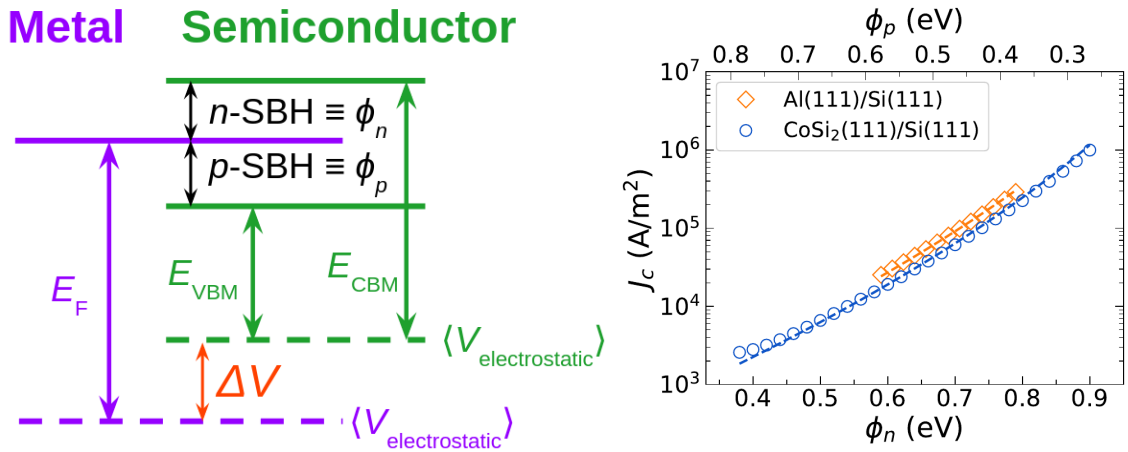

Figure 1. *Left*: Schematic of *n*- and *p*-type Schottky barrier height (SBH) determination from the metal Fermi level E_F, semiconductor valence-band maximum E_{VBM} and conduction-band minimum E_{CBM}, and metal-semiconductor potential alignment ΔV. *Right:* Estimated Josephson critical current density J_c as a function of SBH, shown for Si barrier thickness of 6 nm (diamonds and circles), along with fits to the tunneling probability for a rectangular barrier (dashed curves).

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Supplementary Information

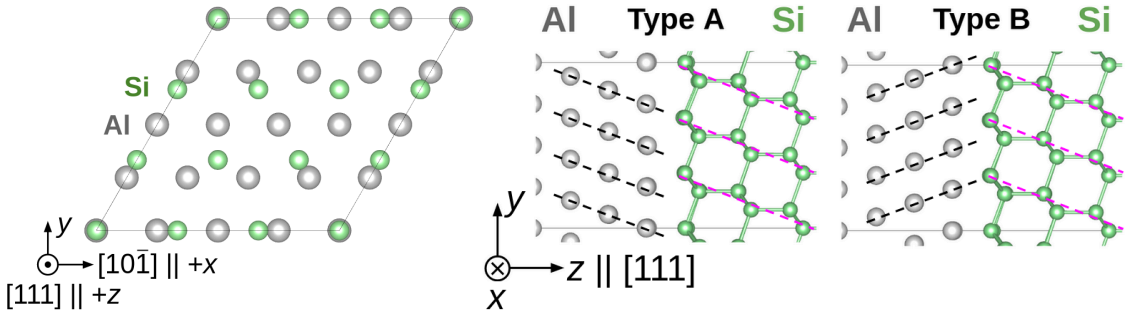

Figure S1. Al(111)/Si(111) structure. *Left*: cross section of the (111) plane, showing 4-to-3 Al-to-Si ratio. *Right*: two different relative orientations between Al and Si (dashed lines) considered.

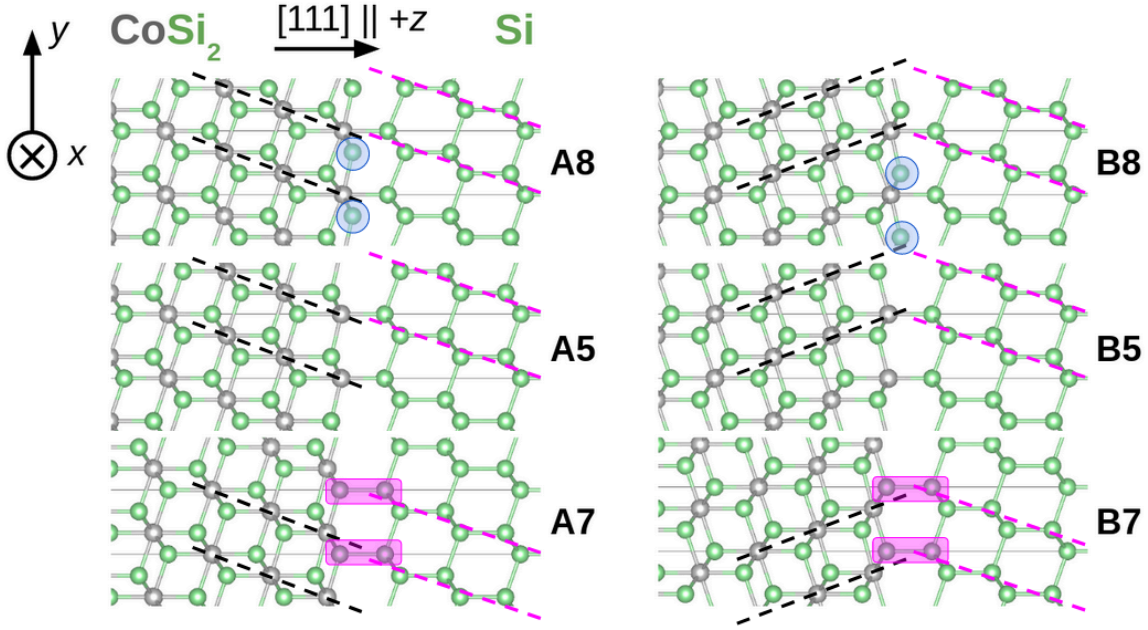

Figure S2. Six structures of lattice-matched $CoSi_2$(111)/Si(111) considered, based on the bonding pattern across the interface and the relative orientation between $CoSi_2$ and Si.

Interface	**Structure**	ϕ_p **(eV)**	ϕ_n **(eV)**	J_c **(A/m^2)**				
				5 nm	**6 nm**	**7 nm**	**10 nm**	**20 nm**
Al/Si	A	0.58	0.59	3×10^5	2×10^4	2×10^3	2	10^{-10}
	B	0.58	0.59	3×10^5	2×10^4	2×10^3	2	10^{-10}
$CoSi_2$/Si	A5	0.41	0.76	9×10^5	1×10^5	2×10^4	46	10^{-7}
	B5	0.41	0.76	9×10^5	1×10^5	2×10^4	46	10^{-7}
	A7	0.68	0.48	7×10^4	6×10^3	4×10^2	0.2	10^{-12}
	B7	0.54	0.63	3×10^5	3×10^4	3×10^3	3.5	10^{-9}
	A8	0.79	0.38	4×10^4	3×10^3	2×10^2	0.05	10^{-13}
	B8	0.56	0.61	2×10^5	2×10^4	2×10^3	2.4	10^{-11}

Table S1. *p*- and *n*-type Schottky barrier heights (ϕ_p and ϕ_n) of all Al(111)/Si(111) and $CoSi_2$(111)/Si(111) structures considered, along with estimated Josephson critical current densities (J_C) for various Si barrier thicknesses of 5–20 nm.

Interface	**Structure**	f_q **(GHz)**				
		5 nm	**6 nm**	**7 nm**	**10 nm**	**20 nm**
Al/Si	A	32	10	3.5	0.1	10^{-6}
	B	32	10	3.5	0.1	10^{-6}
$CoSi_2$/Si	A5	59	23	9.3	0.6	10^{-4}
	B5	59	23	9.3	0.6	10^{-4}
	A7	17	5.0	1.5	0.04	10^{-7}
	B7	31	11	3.8	0.2	10^{-6}
	A8	12	3.4	0.9	0.02	10^{-8}
	B8	29	9.8	3.4	0.1	10^{-6}

Table S2: Corresponding estimated qubit resonant frequencies f_q.