

SUPPLEMENTARY INFORMATION for

Revealing the Role of Interface Disorder in Modulating Critical Current Density of Josephson Junctions

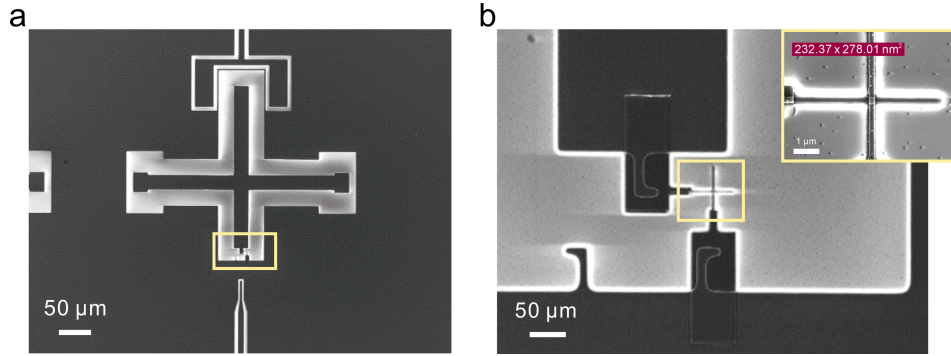
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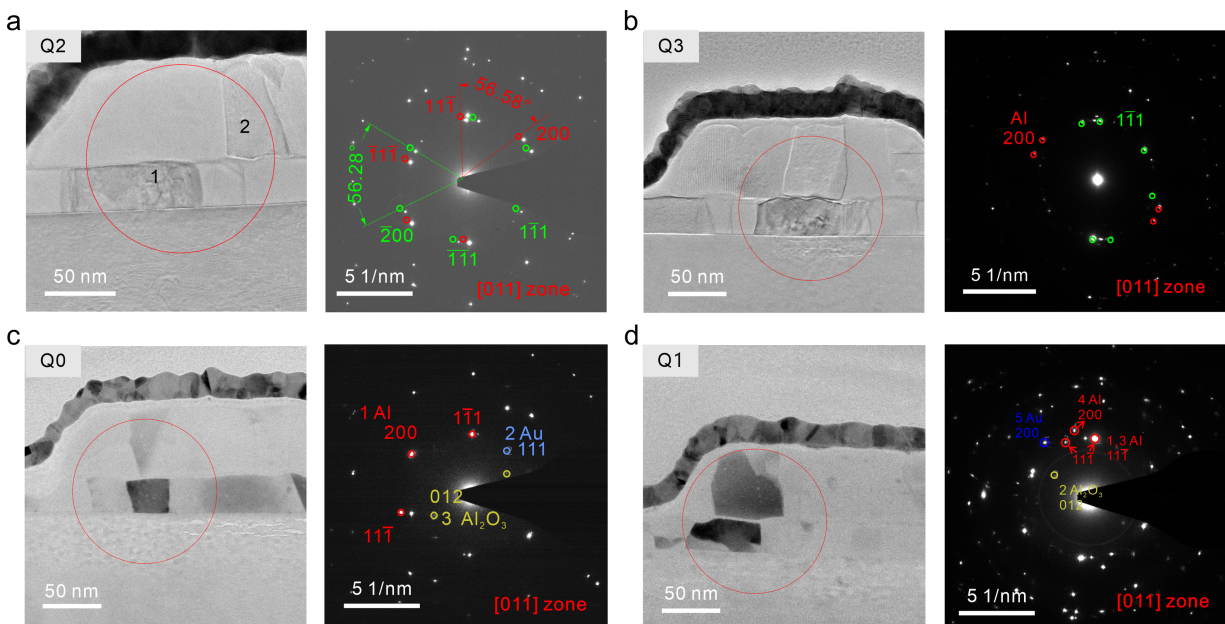
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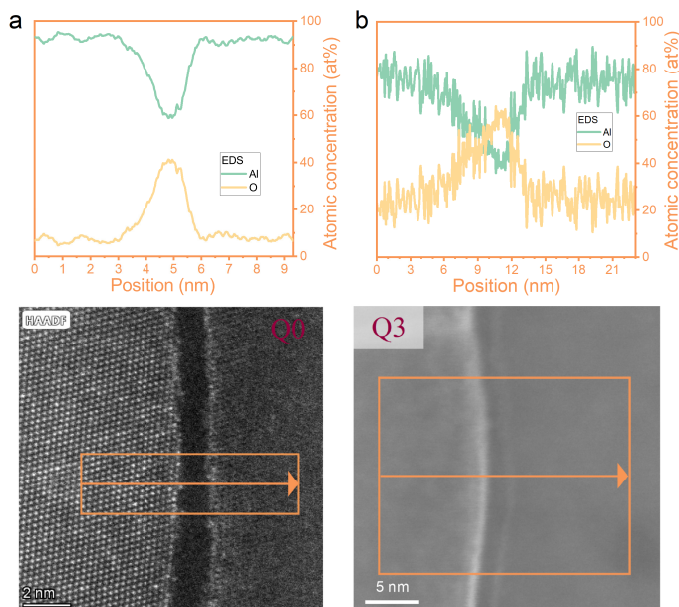
Supplementary Fig. 1. Overall experimental characterization images of an 8-qubit chip. **a-b** Scanning electron microscopy (SEM) images of one of the four qubits and a Josephson junction (JJ) in it. The upper right corner of **b** shows an enlarged view of the JJ.

* The first two authors contributed equally.

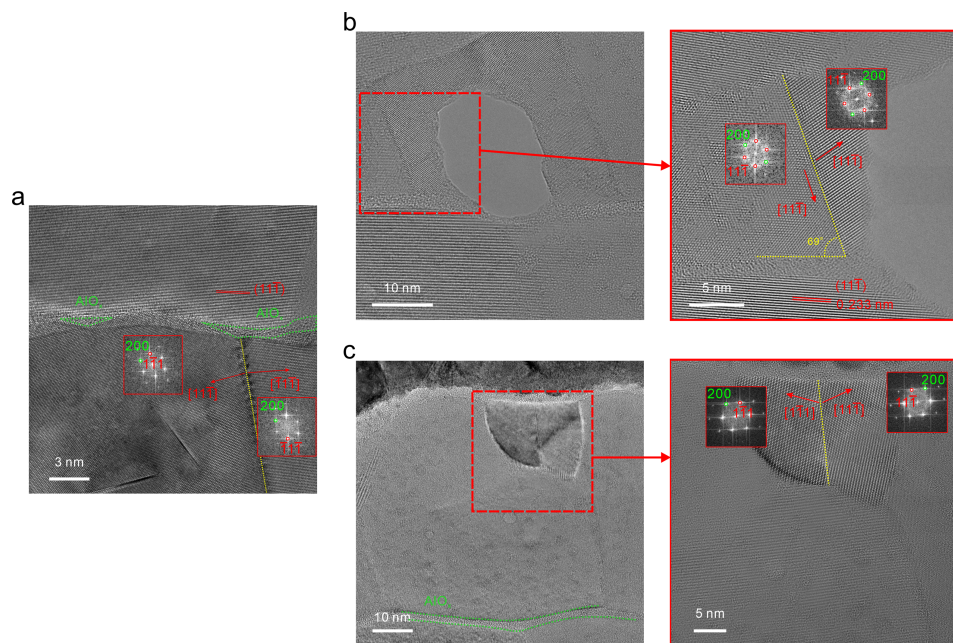
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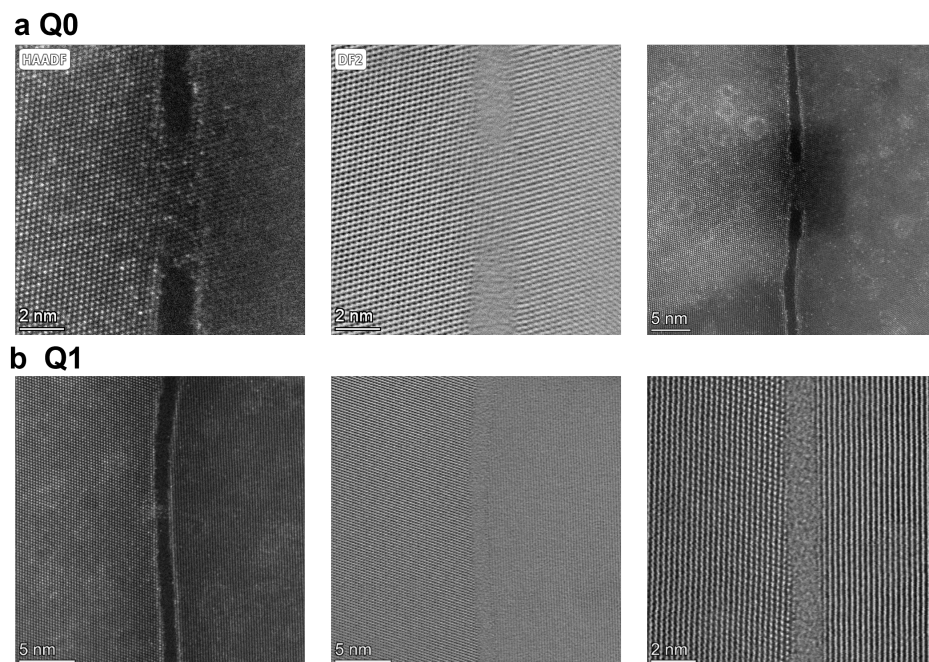
Supplementary Fig. 2. Enlarged transmission electron microscopy (TEM) images and their corresponding selected area electron diffraction (SAED) patterns of the cross-section junctions in **a** Q2, **b** Q3, **c** Q0, and **d** Q1.



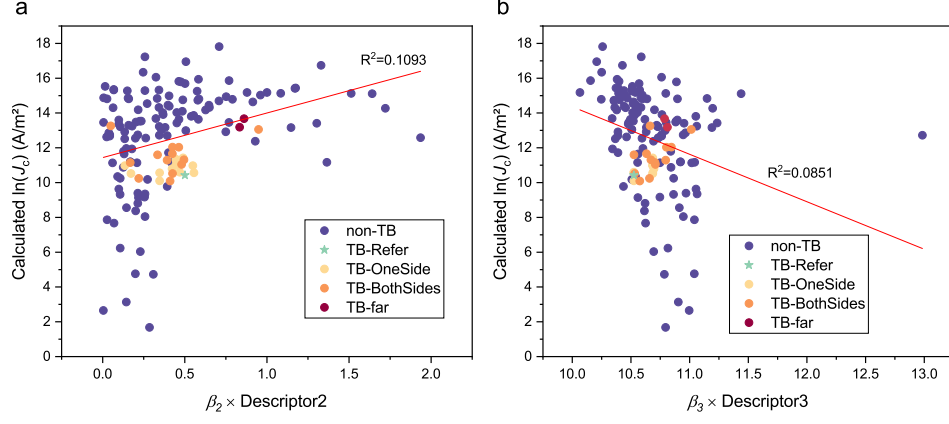
Supplementary Fig. 3. Energy dispersive X-ray spectroscopy (EDX) line scan results near the barrier in JJ of **a** Q0 and **b** Q3 showing Al and O concentrations.



Supplementary Fig. 4. Schematic representations of atomic arrangements at the grain boundaries of **a** Q3, **b** Q0, and **c** Q1.



Supplementary Fig. 5. HAADF, DF, and BF images of tunnel layers in **a** Q0 and **b** Q1 after irradiation during single-photon energy spectroscopy.



Supplementary Fig. 6. Data distributions of **a** $\beta_2 \times \text{Descriptor2}$ and **b** $\beta_3 \times \text{Descriptor3}$ in Equation (2) with respect to calculated $\ln(J_c)$.

Details of NEGF-DFT method for conductance calculation: In the NEGF-DFT method, a transmission function $T(E)$ is expressed in terms of a single Green function and spectral density function, which collectively describes the coupling between device components:

$$T(E) = \text{tr} \left[G^R(E) \Gamma_l(E) G^A(E) \Gamma_r(E) \right], \quad (\text{S1})$$

where $\Gamma_l(E) = i \left[\Sigma_l^R(E) - \Sigma_l^A(E) \right]$ is a spectral density function, and $\Sigma_l^R(E)$ ($\Sigma_l^A(E)$) is the retarded (advanced) self-energy of the electrode l . G^R and G^A denote the retarded and advanced Green's functions of the model, respectively.

$$G^{R,A}(E) = [ES - H - \Sigma^{R,A}]^{-1}, \quad (\text{S2})$$

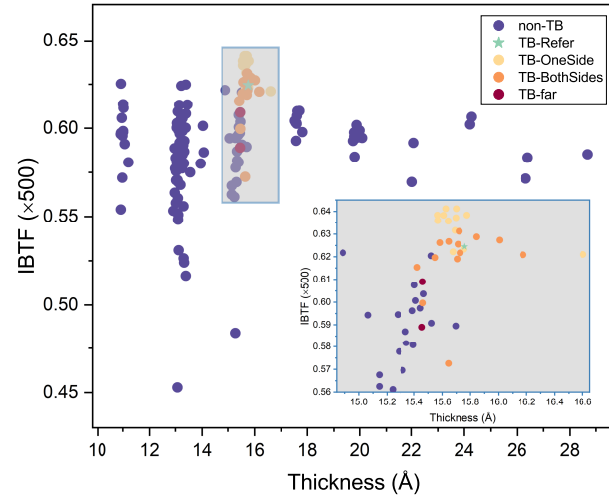
where H is the Hamiltonian matrix of the system, Σ^R and Σ^A denote the delayed and overrunning self-energy, respectively. G^R can be calculated from a matrix transformation using $G^A = (G^R)^\dagger$. S is the overlap matrix due to orbital non-orthogonality. Conductance G is given by [1, 2]:

$$G = G_0 \int dE \frac{f_l(E) - f_r(E)}{eV_r - eV_l} T(E), \quad (\text{S3})$$

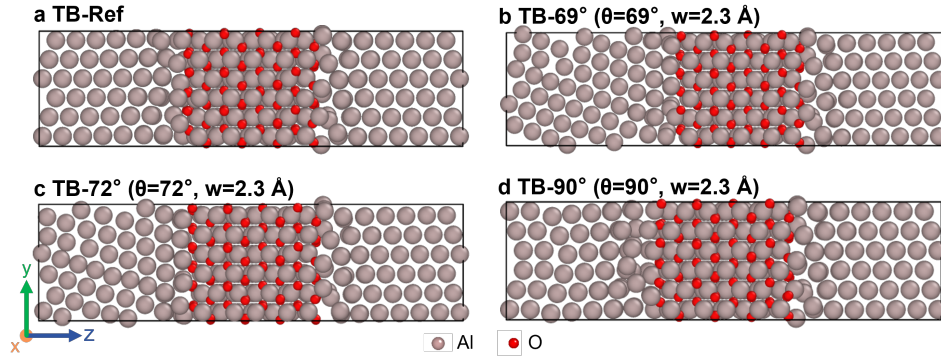
where $G_0 = 2e^2/h = 7.75 \times 10^{-5}$ S is the quantum conductance, h is Planck constant, and e is electron charge. $f_l(E) - f_r(E)$ and $V_r - V_l$ are the differences in the Fermi distributions and the bias applied to the left and right electrodes, respectively.

REFERENCES

- [1] Landauer, R. Electrical resistance of disordered one-dimensional lattices. *Philos. Mag.* **21**, 863–867 (1970) .
- [2] Meir, Y. & Wingreen, N. S. Landauer formula for the current through an interacting electron region. *Phys. Rev. Lett.* **68**, 2512–2515 (1992) .



Supplementary Fig. 7. Relationship between the barrier thickness and IBTF. The inset shows an enlarged view of the area with a thickness of around 16 Å.



Supplementary Fig. 8. Atomic structure diagrams. **a** TB-Ref, and **b-d** three TB-OneSide models. The last three models correspond to TB-OneSide models with angles of 69°, 72°, and 90°, where all have a TB width of 2.3 Å. The atoms along Z direction sequentially belong to the lower Al, Al- AlO_x interface, AlO_x , AlO_x -Al interface, and upper Al region.

Supplementary Table 1. Definition and abbreviation of the primary features

Description	Name	Abbreviation
Cross-sectional area	Area	S
Barrier thickness	Thickness	W
Number of Al atoms	NumAl(_Left, _Right)	NA, NAl, NAr
Number of O atoms	NumO(_Left, _Right)	NO, NOl, NOr
Integral of total radial distribution function	A_RDF	AR
Integral of parital radial distribution function	A_RDF[−AlAl, −AlO, −OO]	AR ^{AlAl,AlO,OO}
Al:O stoichiometric ratios	Stoich(_Left, _Right)	SI, SI _l , SI _r
Average coordination number	AvgCN(_Left, _Right)[−AlAl, −AlO, −OAl, −OO]	ACN ^{AlAl,AlO,OAl,OO} , ACN _l ^{AlAl,AlO,OAl,OO} , ACN _r ^{AlAl,AlO,OAl,OO}
Average bond length	AvgBondLen(_Left, _Right)[−AlAl, −AlO]	ABL ^{AlAl,AlO} , ABL _l ^{AlAl,AlO} , ABLR ^{AlAl,AlO}
Standard deviation of bond length	StdBondLen(_Left, _Right)[−AlAl, −AlO]	SBL ^{AlAl,AlO} , SBL _l ^{AlAl,AlO} , SBL _r ^{AlAl,AlO}
Average bond angle	AvgBondAngle(_Left, _Right)[−AlAlAl, −AlAlO, −AlOAl, −OAlO]	ABA ^{AlAlAl,AlAlO,AlOAl,OAlO} , ABAl ^{AlAlAl,AlAlO,AlOAl,OAlO} , ABAr ^{AlAlAl,AlAlO,AlOAl,OAlO}
Standard deviation of bond angle	StdBondAngle(_Left, _Right)[−AlAlAl, −AlAlO, −AlOAl, −OAlO]	SBA ^{AlAlAl,AlAlO,AlOAl,OAlO} , SBAl ^{AlAlAl,AlAlO,AlOAl,OAlO} , SBAr ^{AlAlAl,AlAlO,AlOAl,OAlO}
Mass density	MassDen(_Left, _Right)	MD, MD _l , MD _r
Number density	NumDen(_Left, _Right)[−Al, −O]	ND ^{Al,O} , ND _l ^{Al,O} , ND _r ^{Al,O}

Note: Here, ‘[]’ indicates that only one option can be selected, while ‘()’ indicates that an option may be omitted or exactly one can be chosen. In this paper, “Left” and “Right” denote the left and right interfaces in the Al-AlO_x-Al atomic model (or more specifically, the lower Al-AlO_x and upper AlO_x-Al interfaces).

Supplementary Table 2. Primary features and RMSE value distribution by SISSO models with different feature complexities and dimensions

Complexity, Dimension	RMSE (Å/m ²)	Primary features
5,3	0.6581	ABAl ^{AlAlAl} , ACN _l ^{OO} , ACN _l ^{AlO} , ACN _r ^{OAl} , SBAr ^{AlAlO} , SBAr ^{OAlO} , ND _r ^{Al} , NO _r
6,3	0.6513	ABAl ^{AlAlAl} , ACN _l ^{AlO} , ACN _l ^{OO} , ND _r ^{Al} , NO _r , SBAl ^{OAlO} , SBAr ^{AlAlO} , SBAr ^{OAlO} , SBL _l ^{AlO} , SBL _r ^{AlAl}
7,3	0.6577	ABAl ^{AlAlAl} , ACN _l ^{AlO} , ACN _l ^{OO} , ACN _r ^{AlAl} , ACN _r ^{OAl} , ND _r ^{Al} , SBAl ^{OAlO} , SBAr ^{AlAlO} , SBAr ^{OAlO}
6,2	0.7190	ABAl ^{AlAlAl} , ACN _l ^{AlO} , ACN _l ^{OO} , ND _r ^{Al} , NO _r , SBAr ^{OAlO}
5,2	0.7203	ACN _l ^{AlO} , ACN _l ^{OO} , ACN _r ^{OAl} , ND _r ^{Al} , NO _r , SBAr ^{AlAlO} , SBAr ^{OAlO}
7,2	0.7272	ACN _l ^{AlO} , ACN _l ^{OO} , ACN _r ^{AlAl} , ACN _r ^{OAl} , ND _r ^{Al} , SBAl ^{AlAlAl} , SBAl ^{OAlO} , SBAr ^{OAlO}
4,3	0.7312	ACN _l ^{AlAl} , ACN _l ^{OO} , ACN _r ^{AlAl} , ACN _r ^{OAl} , SBAl ^{AlAlAl} , SBAl ^{OAlO} , SBAr ^{AlAlO} , SBAr ^{OAlO} , SBL _l ^{AlO}
3,3	0.7611	ACN _l ^{AlO} , ACN _l ^{OO} , ACN _r ^{OAl} , SBAl ^{AlAlAl} , SBAl ^{OAlO} , SBAr ^{AlAlO} , SBAr ^{OAlO}

Note: The corresponding mathematical formulas and their fitting coefficients can be found in Supporting Information.