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# Supporting information

## Multilevel Oxygen-vacancies Conductive Filaments in the β-$Ga_2O_3$ Based Resistive Random Access Memory

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**Table S1**. The defect formation energies of $V_O$s with different charge states at $E_F = 0$ eV under the O-rich condition in the β-$Ga_2O_3$ supercells with 120, 160, and 300 atoms.

| supercell | 0 charge state | | | +2 charge state | | |
|---|---|---|---|---|---|---|
| | $V_{O1}$ | $V_{O2}$ | $V_{O3}$ | $V_{O1}$ | $V_{O2}$ | $V_{O3}$ |
| 120 atoms | 1.2967 | 0.3729 | 0.5083 | 3.6041 | 4.0112 | 4.2763 |
| 160 atoms | 1.2944 | 0.3721 | 0.5064 | 3.6038 | 4.0093 | 4.2711 |
| 300 atoms | 1.2950 | 0.3709 | 0.5073 | 3.6046 | 4.0106 | 4.2715 |

Supercells of 120, 160, and 300 atoms are employed to verify the convergence of defect formation energies. It can be seen from Table S1 that there is negligible difference (less than 0.01 eV) between the defect formation energies obtained in supercells of 120, 160, and 300 atoms, regardless of the position and charge state of $V_O$. Thus, the 1 × 3 × 2 supercell of 120 atom is used to investigate the properties of defective β-$Ga_2O_3$.

**Table S2**. The defect formation energies (eV) of charged $V_O$s at different $E_F$ (the value of EF is listed in the parentheses) under the O-rich condition and Ga-rich condition.

| | Under the O-rich condition | | | |
|---|---|---|---|---|
| | 0 | +1 | +2 | -3 |
| $V_{O1}$ | 3.61 (2.26 eV) | 3.41 (0 eV) | 1.29 (0 eV) | |
| $V_{O2}$ | 4.03 (2.26 eV) | 2.84 (0 eV) | 0.37 (0 eV) | |
| $V_{O3}$ | 4.28 (2.26 eV) | 2.93 (0 eV) | 0.48 (0 eV) | |
| $V_{Ga1}$ | 4.85 (0 eV) | | | -0.84 (2.26 eV) |
| $V_{Ga2}$ | 5.23 (0 eV) | | | -1.15 (2.26 eV) |
| | Under the Ga-rich condition | | | |
| | 0 | +1 | +2 | -3 |
| $V_{O1}$ | 0.50 (2.26 eV) | 0.27 (0 eV) | -1.81 (0 eV) | |
| $V_{O2}$ | 0.92 (2.26 eV) | -0.28 (0 eV) | -2.74 (0 eV) | |
| $V_{O3}$ | 1.17 (2.26 eV) | -0.18 (0 eV) | -2.63 (0 eV) | |
| $V_{Ga1}$ | 9.51 (0 eV) | | | 3.81 (2.26 eV) |
| $V_{Ga2}$ | 9.89 (0 eV) | | | 3.99 (2.26 eV) |

**Table S3**. The calculated Bader charge for neighboring Ga-atoms around different $V_O$ in the β-$Ga_2O_3$ supercell.

| | Pure β-$Ga_2O_3$ | Defective β-$Ga_2O_3$ with $V_O^0$ | | | Defectiveβ-$Ga_2O_3$ with $V_O^{2+}$ | | |
|---|---|---|---|---|---|---|---|
| | | $V_{O1}^0$ | $V_{O2}^0$ | $V_{O3}^0$ | $V_{O1}^{2+}$ | $V_{O2}^{2+}$ | $V_{O3}^{2+}$ |
| $Ga_1$ | 1.75 e | 1.86 e | 1.83 e | 1.82 e | 2.26 e | 2.69 e | 2.61 e |
| $Ga_2$ | 1.68 e | 1.78 e | 1.73 e | 1.73 e | 2.21 e | 2.49 e | 2.47 e |

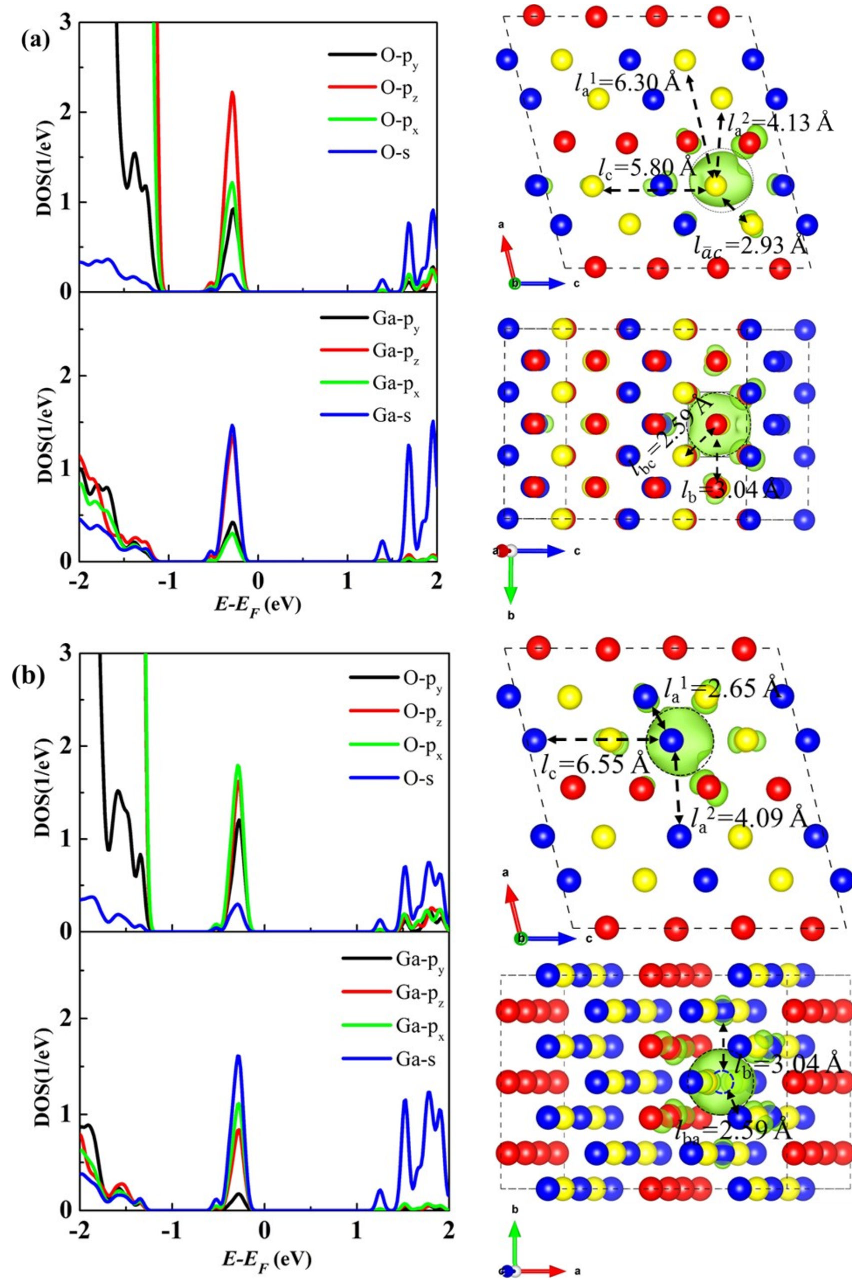


**Figure S2**. Density of states and charge density distributions of (a) $V_{O2}$ and (b) $V_{O3}$ in β-$Ga_2O_3$, respectively. The marked $l_a$, $l_b$, and $l_c$ are respective the distance between $V_O$ and the O atom at its equivalent site along the a, b, and c direction.

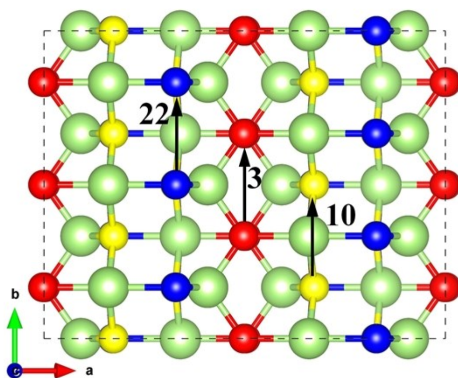


**Figure S3.** The migration pathways of O-vacancies along the b direction. The path 3, 10 and 22 are respective the migrations of $V_{O1}$, $V_{O2}$ and $V_{O3}$, respectively.