**Deciphering the molecular mechanism of water boiling at heterogeneous interfaces**

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**Supplementary Informatio n**



**Figure S1.** Radial distribution function of the zirconia interface atoms (Zr, Ozr) with the oxygen and hydrogen atoms of the water molecules for the (001) and (-111) interface planes. In both interface planes, the water dipoles are oriented with the hydrogen atom being closer to the interface.



**Figure S2.** Density profile in fluid phase normal to zirconia interface at hydrophobic (001) and hydrophilic (-111) zirconia surface faces. In the hydrophilic (-111) interface plane, a hydrogen pre-peak close to the solid interface is evident, indicating the formation of hydrogen bonds between the water and solid atoms.

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| **(a)** | **(b)** | **(c)** |

**Figure S3.** Contact angle estimation on water vapor bubble embedded into condensed phase at (‑111) the interface.

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|  |  |
| **(a)** | **(b)** |

**Figure S4.** Average of Hamiltonian derivatives (usl(LJ) and usl(C))and work of adhesion (Wsl) for a) the zirconia (-111) interface plane at 298.15K and 396.15K and b) the zirconia (001) interface plane at 298.15K and 396.15K respectively. The work of adhesion (Wsl) at κ=1 on the LJ coupling parameter case was used as the initial value for the work of adhesion using the Coulomb coupling parameter. The cumulative Wsl (at λ equal to 1.0) of the Coulomb coupling parameter was applied in the Young-Dupré equation to calculate the water contact angle.



**Figure S5**. Water density profile evolution during the initial stage heterogeneous water nucleate boiling in contact with the (-111) interface of mZrO2. The two independent density profiles indicate a thin adsorbed water layer (6-8Å) on the hydrophilic interface. The almost constant increase of the box size along z-distance (bottom graph) indicates the trajectory decorrelation from the artificially generated pathway (the initial stage of heterogeneous water nucleate boiling, explosive boiling).



**Figure S6.** Parallel mean square displacement (MSD) divided by the survival probability (SP) for specific water layers from the zirconia interface at (-111) face. The parallel MSD is defined as the average MSD values in x and y directions.



**Figure S7.** Potential of mean force (PMF) profile of a hydrophobic particle normal to zirconia interface at (001) and (-111) surface faces.