Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Atomic-scale Structure of Misfit Dislocations in CeO_2/MgO Heterostructure and Thermodynamic Stability of Dopant-defect Complexes at the Heterointerface

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Supplementary Information

Figure S1. *Illustration of few stable* M–$V_O^{\cdot\cdot}$–M *clusters with 1NN–2NN arrangement in the vicinity of Layer-1. Figure details are similar to* ***Figure 4*** *in the main manuscript. For each dopant species, the energy (eV) for a particular cluster of the respective number is given in* ***Table S1****. Color scheme for Ce, Mg, and O ions is shown below the figure.*

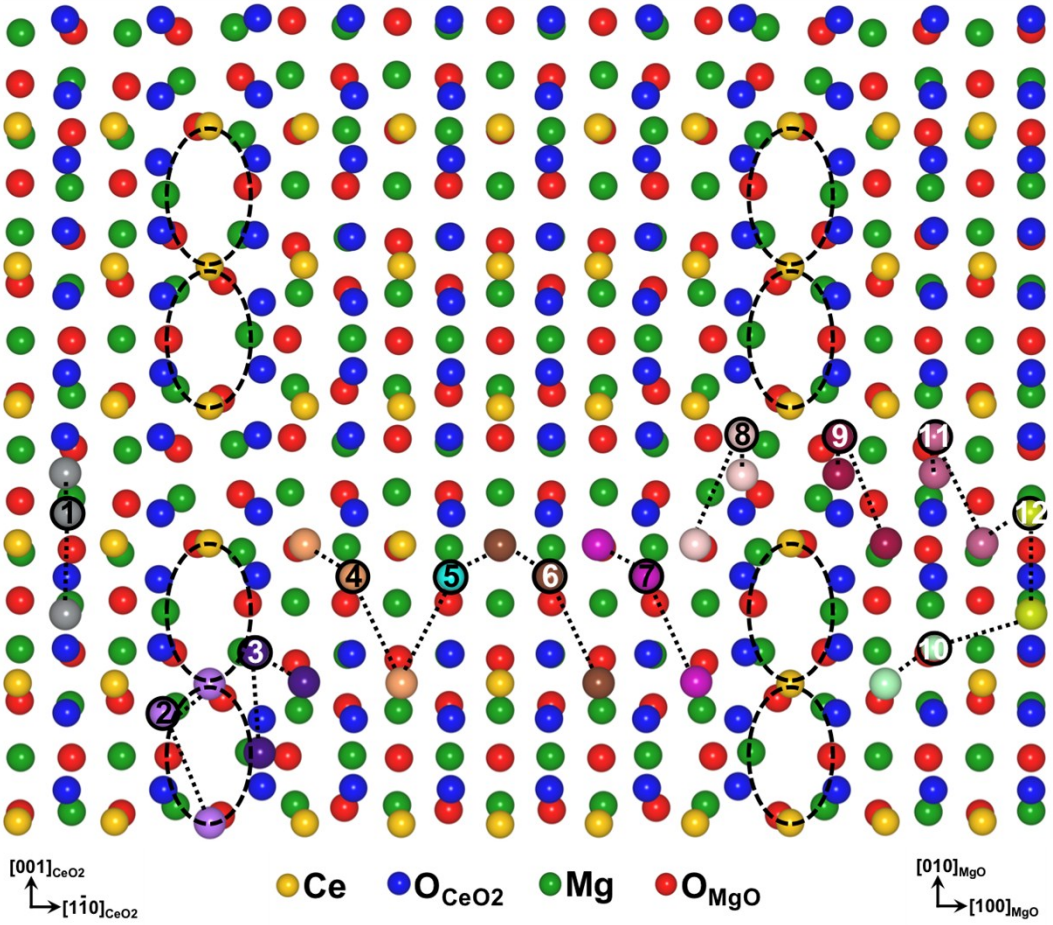

Table S1. *For various trivalent dopants, energy (eV) for the respective* M–$V_{\ddot{O}}$–M *cluster number with 1NN–2NN arrangement in Layer-1, as displayed in* ***Figure S1****. Energies are scaled so that 0.0 eV indicates the most favorable cluster arrangement.*

***M*–$V_{\ddot{O}}$–*M* cluster number**	**Y (eV)**	**Gd (eV)**	**Sm (eV)**	**La (eV)**
1	3.72	3.94	4.08	4.71
2	2.95	3.17	3.30	3.64
3	2.92	3.09	3.23	3.75
4	0.54	0.76	0.86	2.01
5	0.34	0.47	0.57	0.89

6	0.32	0.46	0.55	0.85
7	0.43	0.59	0.74	1.03
8	3.14	3.50	3.66	4.25
9	1.02	1.20	1.24	1.56
10	0.34	0.50	0.58	0.82
11	0.41	0.44	0.44	0.56
12	2.37	2.44	2.44	2.55