SUPPLEMENTARY MATERIAL

In Table I, we describe the local environment of the defects studied in this work through the number of O atoms in the first-neighbor coordination shell. The associated charge transition levels are also given.

TABLE I. Number of O atoms within the first-neighbor coordination shell of the cation defect and average distance between the cation defect and its nearest neighbor atoms, obtained for both the charge states $q = 0$ and $q = -2$. We used cut-off radii of 2.22 and 2.40 Å for Ga-O and In-O bond lenghts, respectively. The $0/-2$ charge transition levels ($\varepsilon_{0/-2}$) of the identified defects are referred to the CBM of InGaAs.

	$q = 0$		$q = -2$		$\varepsilon_{0/-2}$ (eV)
	#O atoms	$\langle d_{X-\mathrm{O}} \rangle$ (Å)	#O atoms	$\langle d_{X-\mathrm{O}} \rangle$ (Å)	
$\mathrm{In_{Al}}$ (1)	4	2.06	2	2.19	1.03
$\mathrm{In_{Al}}$ (2)	5	2.15	3	2.31	0.98
$\mathrm{In_{Al}}$ (3)	4	2.08	3	2.21	1.12
$\mathrm{In_{Al}}$ (4)	5	2.22	2	2.14	0.57
$\mathrm{In_{Al}}$ (5)	4	2.01	3	2.18	0.61
$\mathrm{In_{Al}}$ (6)	6	2.18	3	2.26	0.78
$\mathrm{Ga_{Al}}$ (1)	4	1.89	2	2.06	1.09
$\mathrm{Ga_{Al}}$ (2)	5	1.98	2	1.86	0.94