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# New insight into the interaction between divacancy and H/He impurity in $Ti_3AlC_2$ by first-principles studies

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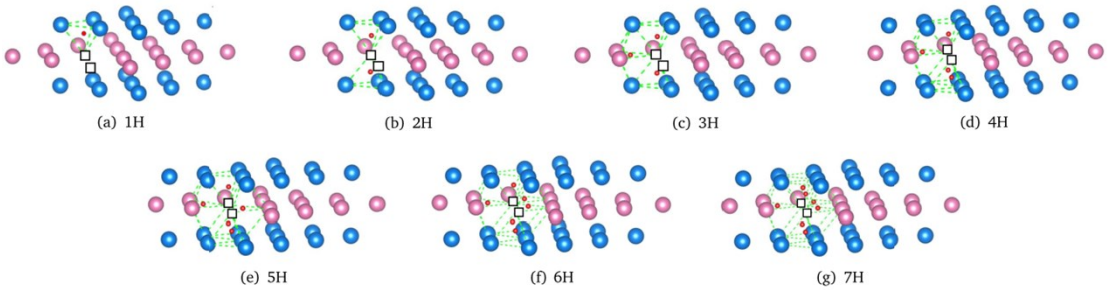


**Fig. S1** Atomic configurations for different numbers of H atoms trapped in the $2V_{Al-Al}$ divacancy. Blue spheres, pink spheres, and red spheres denote Ti atoms, Al atoms and H atoms, respectively. The black squares denote Al vacancies.

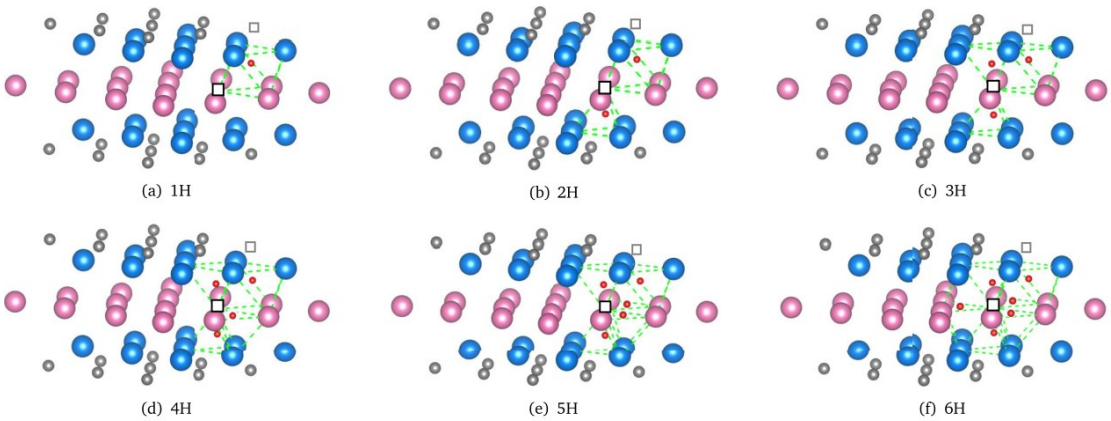


**Fig. S2** Atomic configurations for different numbers of H atoms trapped in the $2V_{Al-C}$ divacancy. Blue spheres, pink spheres, gray spheres, and red spheres denote Ti atoms, Al atoms, C atoms and H atoms, respectively. The black square and gray square denote Al vacancy and C vacancy, respectively.

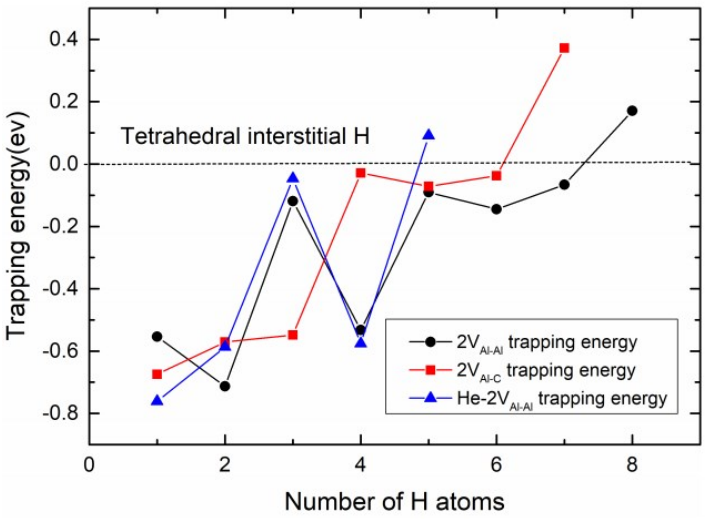


**Fig. S3** Trapping energy for H atom as a function of the number of H atoms trapped by divacancy and He-2V complex in $Ti_3AlC_2$.

**Table S1**

Summary of solution energies, lattice parameters and volume changes with increasing number of trapped H atoms in divacancies and He-2V complex.

| Configuration | $E_s$(ev) | a(Å) | c(Å) | V(Å$^3$) | Δa/a(%) | Δc/c(%) | ΔV/V(%) |
|---|---|---|---|---|---|---|---|
| $Ti_3AlC_2$ | – | 3.0820 | 18.6374 | 1380.20 | – | – | – |
| $2V_{Al-Al}$ | – | 3.0870 | 18.5271 | 1378.33 | 0.1622 | -0.5918 | -0.1355 |
| 1H-$2V_{Al-Al}$ | -0.81 | 3.0888 | 18.5599 | 1379.28 | 0.2206 | -0.4158 | -0.0667 |
| 2H-$2V_{Al-Al}$ | -1.77 | 3.0871 | 18.5818 | 1379.41 | 0.1655 | -0.2983 | -0.0572 |
| 3H-$2V_{Al-Al}$ | -2.04 | 3.0879 | 18.5523 | 1378.09 | 0.1914 | -0.4566 | -0.1529 |
| 4H-$2V_{Al-Al}$ | -2.82 | 3.0857 | 18.5829 | 1378.95 | 0.1201 | -0.2924 | -0.0906 |
| 5H-$2V_{Al-Al}$ | -3.16 | 3.0862 | 18.5486 | 1376.90 | 0.1363 | -0.4765 | -0.2391 |
| 6H-$2V_{Al-Al}$ | -3.55 | 3.0868 | 18.5269 | 1376.01 | 0.1557 | -0.5929 | -0.3036 |
| 7H-$2V_{Al-Al}$ | -3.87 | 3.0867 | 18.5051 | 1374.72 | 0.1525 | -0.7097 | -0.3970 |
| $2V_{Al-C}$ | – | 3.0830 | 18.6025 | 1378.43 | 0.0324 | -0.1873 | -0.1282 |
| 1H-$2V_{Al-C}$ | -0.93 | 3.0825 | 18.6060 | 1378.67 | 0.0162 | -0.0017 | -0.1109 |
| 2H-$2V_{Al-C}$ | -1.75 | 3.0809 | 18.6346 | 1379.33 | -0.0357 | -0.0150 | -0.0630 |
| 3H-$2V_{Al-C}$ | -2.54 | 3.0802 | 18.6506 | 1379.17 | -0.0584 | 0.0708 | -0.0746 |
| 4H-$2V_{Al-C}$ | -2.82 | 3.0814 | 18.6228 | 1377.66 | -0.0195 | -0.0783 | -0.1840 |
| 5H-$2V_{Al-C}$ | -3.14 | 3.0819 | 18.6014 | 1377.01 | -0.0032 | -0.1932 | -0.2311 |
| 6H-$2V_{Al-C}$ | -3.43 | 3.0827 | 18.5743 | 1375.94 | 0.0227 | -0.3386 | -0.3087 |
| He-$2V_{Al-Al}$ | – | 3.0883 | 18.5537 | 1381.20 | 0.2044 | -0.4491 | 0.0725 |
| 1H-He-$2V_{Al-Al}$ | -0.30 | 3.0878 | 18.5693 | 1381.07 | 0.1882 | -0.3654 | 0.0630 |
| 2H-He-$2V_{Al-Al}$ | -1.14 | 3.0871 | 18.6031 | 1382.20 | 0.1655 | -0.1840 | 0.1449 |
| 3H-He-$2V_{Al-Al}$ | -1.41 | 3.0880 | 18.5641 | 1380.07 | 0.1947 | -0.3933 | -0.0094 |
| 4H-He-$2V_{Al-Al}$ | -2.24 | 3.0866 | 18.5808 | 1379.65 | 0.1493 | -0.3037 | -0.0398 |