

Electronic Supplement Information

**Highly efficient catalytic activity for the hydrogen evolution
reaction on the pristine and monovacancy defected WP systems:
A first-principles investigation**

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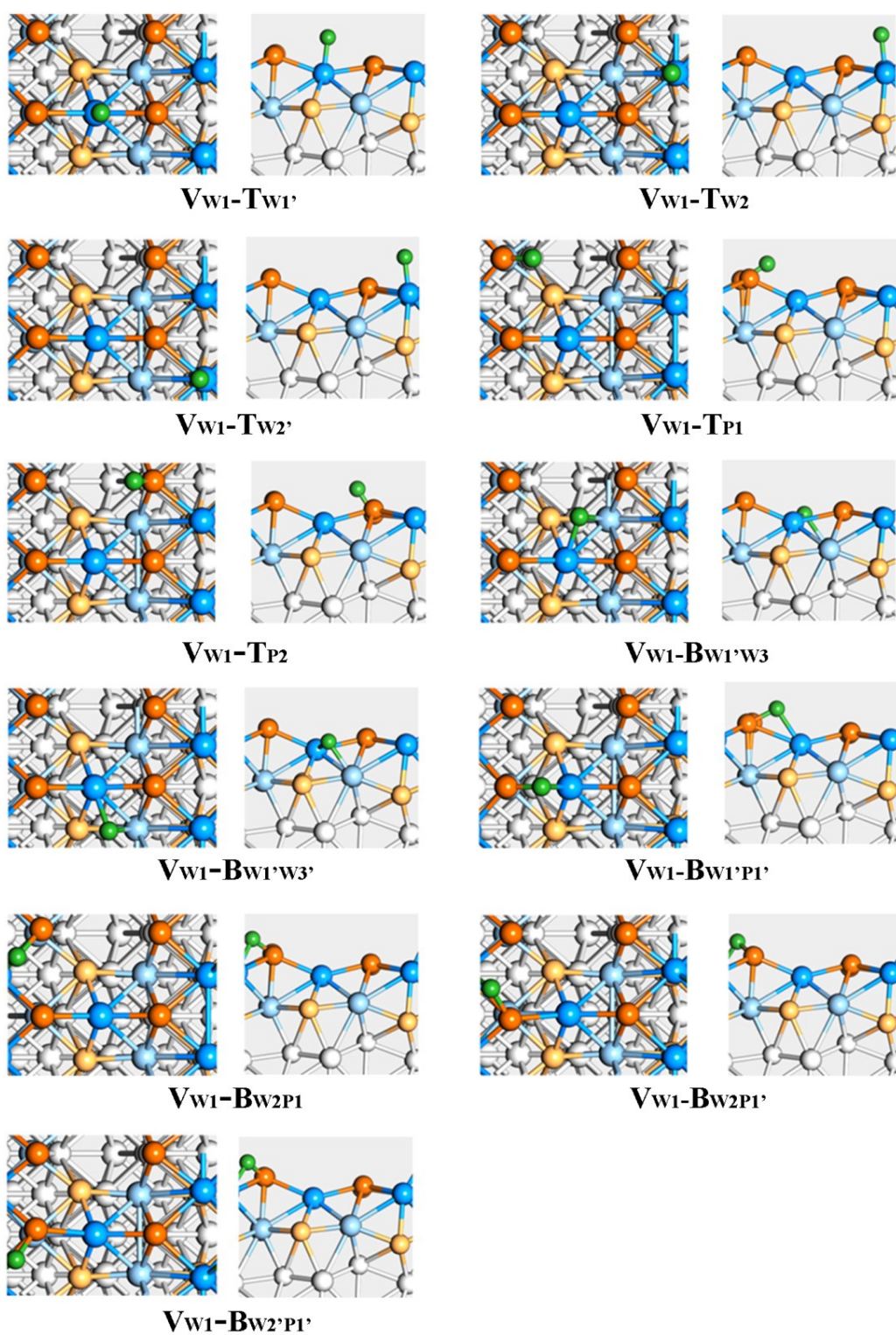


Figure S1. The obtained structures of H* adsorbed on the (101)-V_{w1} surface after relaxation.

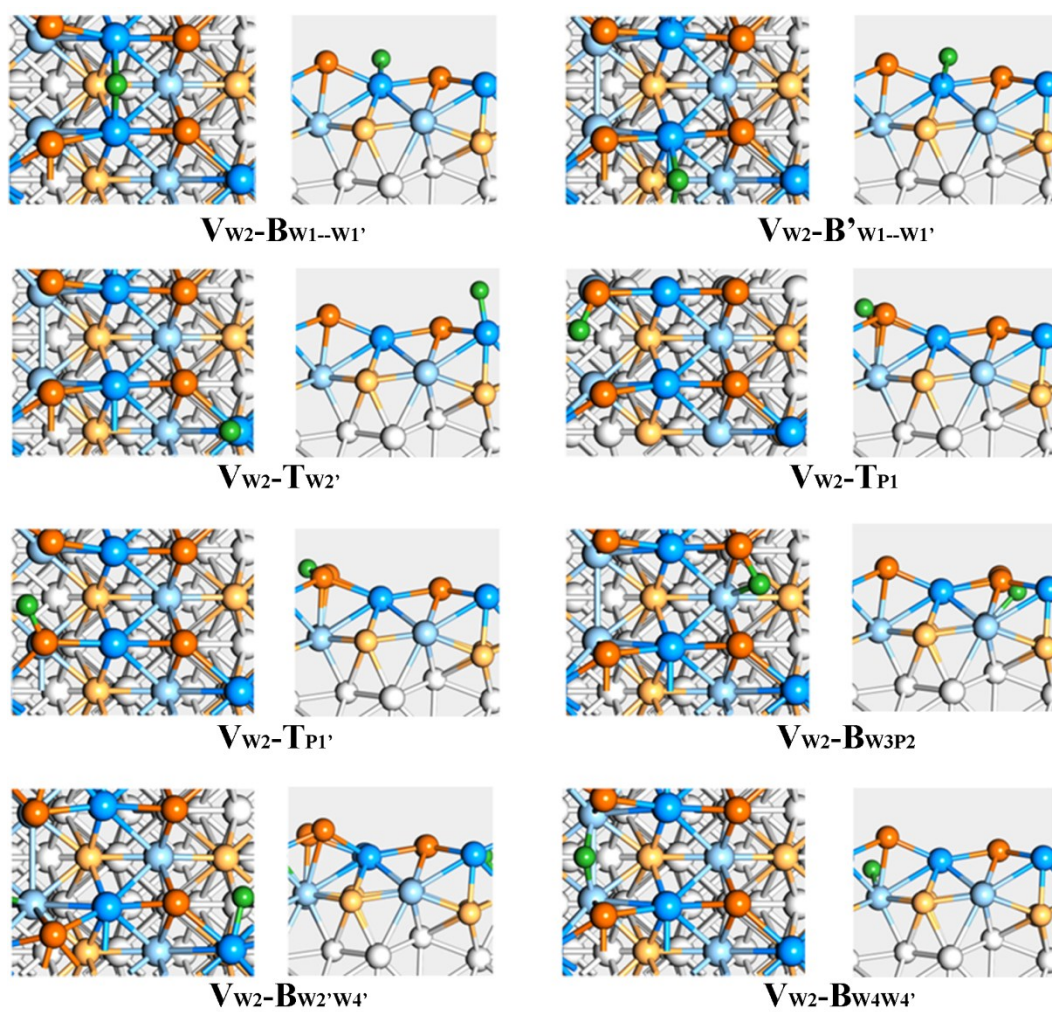


Figure S2. The obtained structures of H^* adsorbed on the (101)- V_{w2} surface after relaxation.

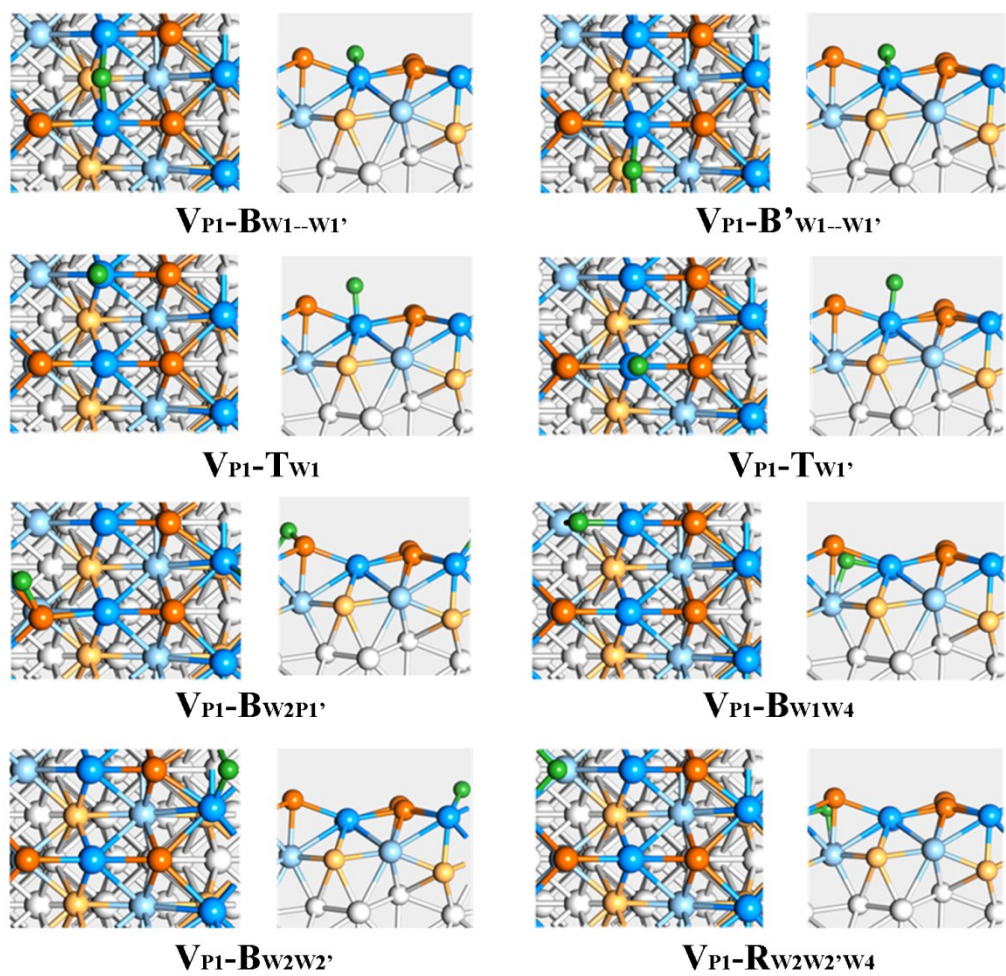


Figure S3. The obtained structures of H* adsorbed on the (101)-V_{p1} surface after relaxation.

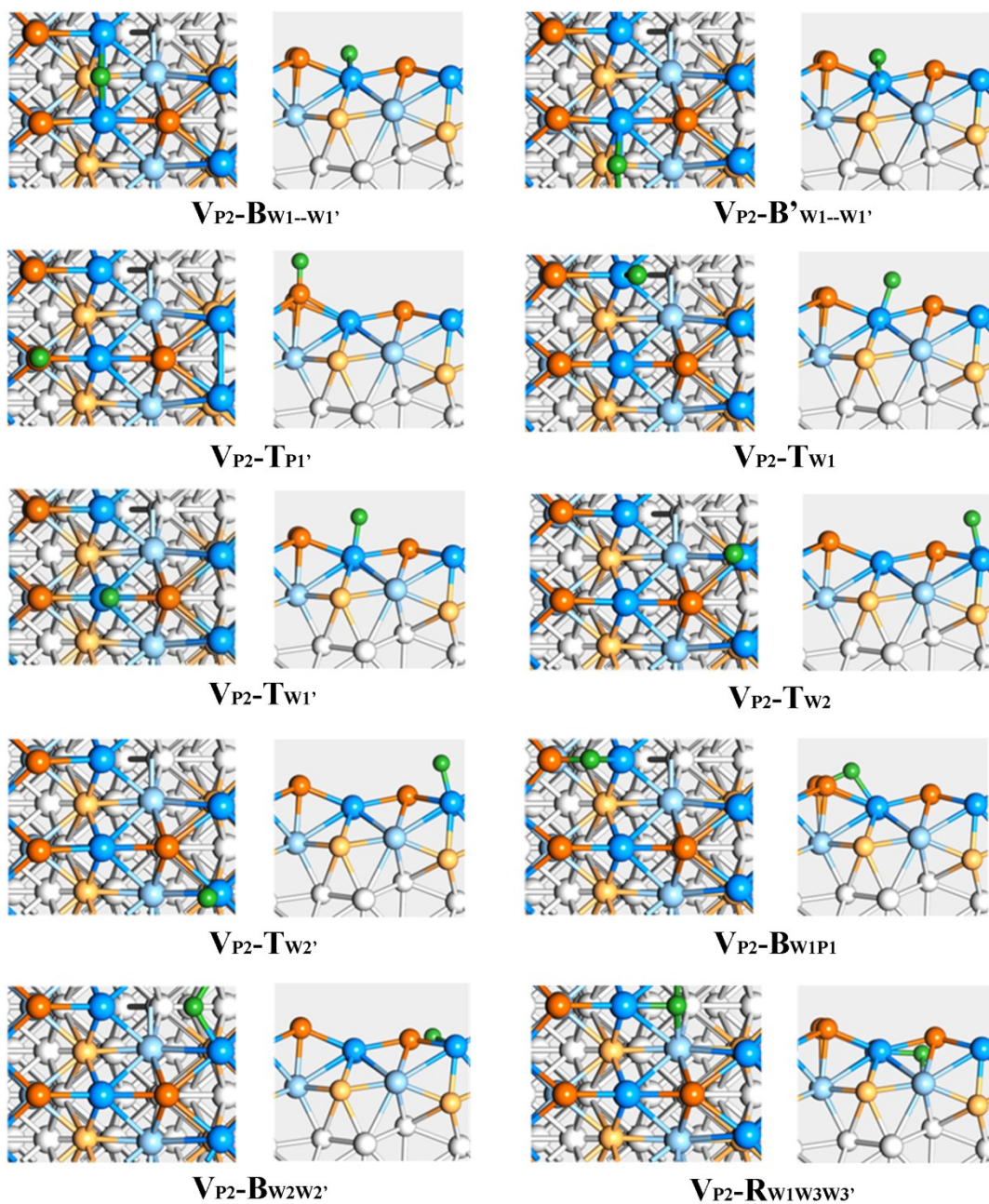


Figure S4. The obtained structures of H* adsorbed on the (101)-V_{p2} surface after relaxation.