Electronic structure and molecular properties of WC

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Molecular properties are the prerequisites needed for understanding the thermodynamic processes during plasma wall interactions (PWI), where the tungsten carbide is the material of choice and WC molecules can participate.

Our long-term goal is the systematic mapping of various spectroscopic states of tungsten carbide. Our approach is different from usual strategy adopted in multireference configuration interaction studies that use the same set of reference orbitals for manifold of states. We aim at elucidating the effect of the reference orbitals on both the spectral and electric properties of low-lying states of WC that can be described adequately by our "standard approach" combining scalar-relativistic Douglas-Kroll-Hess (DKH) Hamiltonian and Coupled Clusters method with Single and Double excitations corrected perturbatively for the Triple excitations (CCSD(T)) and with Restricted Active Space Self-consistent Field method (RASSCF) augmented with multireference perturbation theory (CASPT2).

Comparison with the experimental [1] and previous theoretical [2] data is given.

References

[1] S. M. Sickafoose, A. W. Smith, M. D. Morse, *J. Chem. Phys.* **2002**, *116*, 993.
[2] K. Balasubramanian, *J. Chem. Phys.* **2000**, *112*, 7425.