Ab initio Stellar Astrophysics: Reliable Modeling of Cool White Dwarf Atmospheres

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Over the last decade *ab initio* modeling entered various research fields and proved to be a good tool for predicting various properties of matter under different, even extreme conditions. In our work we apply modern computational chemistry and materials science methods, including density functional theory (DFT), to solve important problems encountered in the modeling of the dense atmospheres of cool white dwarfs ($T_{\rm eff} < 7000\,{\rm K}$). Our work on the revision and improvements of the absorption mechanisms in hydrogen and helium dominated atmospheres resulted in a new set of atmosphere models. By inclusion of Ly-α red wing opacity we successfully fitted the entire spectral energy distributions of known cool DA stars. In the subsequent work we fitted the majority of the coolest stars with hydrogen-rich models. This finding challenges our understanding of the white dwarfs atmospheric evolution. We will show and discuss examples of such fits, including Halo candidates and the cool white dwarf star belonging to the binary system with pulsar PSR J0437-4715 and discuss the implications. The two problems important for the understanding of cool white dwarfs are the behavior of negative hydrogen ion and molecular carbon in a fluid-like, helium dominated medium. Using *ab initio* methods we investigate the stability and opacity of these two species in dense helium. We will show that the negative hydrogen ion does not undergo pressure ionization up to a density of $4\,{\rm g/cm^3}$, but its bound-free absorption edge moves to the shorter wavelengths with increasing helium density. Our investigation of C_2 indicates that the absorption features observed in the peculiar, cool DQ white dwarfs resemble the absorption of perturbed C_2 in dense helium, however the photospheric densities needed to explain the observed Swan bands shifts are one order of magnitude smaller than the ones predicted by the current atmosphere models.