Understanding the Oldest White Dwarfs: Atmospheres of Cool WDs as Extreme Physics Laboratories

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Reliable modeling of the atmospheres of cool white dwarfs is crucial for understanding the atmospheric evolution of these stars and accurate white dwarfs cosmochronology. Over the last decade *ab initio* modeling entered various research fields and has been successful in predicting properties of various materials and matter under extreme conditions. In our work we apply the modern electronic structure methods, mainly density functional theory, to solve important problems encountered in various research fields, including dense, fluid like atmospheres of cool white dwarfs. In many cases the investigated physical regimes are difficult or even impossible to access by experimental methods, and the first principles quantum mechanical calculations are the only tools available for investigation. Using modern methods of computational chemistry we investigate the atmospheres of helium-rich, old white dwarfs. Such atmospheres reach extreme, fluid like densities (up to grams per cm^3) and represent an excellent laboratory for high temperature and pressure physics and chemistry. We show our results for the stability and opacity of H^- and C_2 in dense helium and the implications of our work for understanding cool white dwarfs. We also present the fits by our improved atmosphere models to the recently obtained spectral energy distributions of various cool white dwarfs, and discuss the impact of derived atmospheric compositions on the understanding of the atmospheric evolution of these stars and the stellar systems to which these stars belong.