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

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Outline

White dwarfs atmosphere modeling
- Atmospheres of cool white dwarfs:
- Why *ab initio* modeling is so important?
- our improvements

Performance of the models
- Fits to the SEDs of cool WDs (*including Halo candidates*)
- WD in a binary system with a pulsar

Examples of *ab initio* investigation
- Stability of H\(^-\) in dense helium
- Investigation of the spectroscopic properties of C\(_2\) in dense He (*solving the “peculiar” DQs problem*)
Atmospheres of cool WDs

Important
- Their composition determine the cooling rates and ages at the ends of WDs cooling sequences

Problematic
- H-lines detectable down to $T_{\text{eff}} \sim 5000\,\text{K}$
- He-rich atm. is a fluid, not an ideal gas!

“For simplicity, we have neglected all non-ideal effects, since these effects are poorly understood”

*Kilic et al., 2010, ApJS*
Why *ab initio* modeling?

**Because:**

- Development of the QM methods, software and hardware allows for first principle simulations of matter under extreme conditions (*like WDs atmospheres*)

*Ab initio* models for:

- Non-ideal abundances of species
- Opacity of strongly correlated, fluid media
Our improvements

<table>
<thead>
<tr>
<th>Current state</th>
<th>Our improvements</th>
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<tbody>
<tr>
<td>Radiative transfer for planar non-refractive atmosphere</td>
<td>Radiative Transfer Equation in a refractive medium</td>
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<td>Currently, the following species are included: $\text{H}_2$, $\text{H}$, $\text{H}^+$, $\text{H}_2^+$, $\text{H}_3^+$, $\text{H}^-$, $\text{He}$, $\text{He}_2^+$, $\text{He}^+$, $\text{HeH}^+$, $\text{e}^-$, but chemistry is that of ideal gas (except ionization equilibrium of He)</td>
<td>The non-ideal chemical equilibrium abundances of species: $\text{H}$, $\text{H}_2$, $\text{H}^-$, $\text{He}$, $\text{He}^+$, $\text{He}_2^+$, $\text{e}^-$</td>
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<td>Dilute gas photo absorption cross-sections and chemistry</td>
<td>A revision of the most important sources of opacities in helium-rich WD atmospheres: $\text{He}^-$ ff, $\text{H}^-$ bf</td>
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<td>Flux excess in the model spectra of hydrogen atmosphere white dwarfs</td>
<td>Found the missing absorption mechanism at short wavelengths (Ly(\alpha))</td>
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<td>Unknown nature of “peculiar” DQs</td>
<td>Density induced spectral distortion of $\text{C}_2$ bands</td>
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Performance: fits to the SEDs of cool WDs

Majority of cool DC stars have hydrogen rich atmospheres?!
**Performance: WDs Halo candidates**

Hall et al., 2008, AJ, 136, 76

Kilic et al., 2010, ApJL, 715, L21

![Graph showing synthetic spectra of pure H, pure He, and mixed H/He models](image)

Fig. 5.— Synthetic spectra of pure H, pure He and mixed H/He models, all assuming log g = 8. Fits to all data yield $T_{\text{eff}} \approx 3800$ K for pure H (solid green) and $T_{\text{eff}} = 4381$ K for pure He (solid blue). Fits to optical data only yield $T_{\text{eff}} = 3450$ K for pure H (dotted green) and $T_{\text{eff}} = 3860$ K for pure He (dotted blue). Helium-dominated models with $T_{\text{eff}} = 3500$ K are shown by the red lines, with hydrogen contents as follows: log H/He = −3 (solid), −1 (dash-dotted), −5 (dotted) and −5.5 (dashed).
WD in a binary system with a pulsar

Binary system: pulsar PSR J0437-4715 + WD

- Pulsar points
- $\text{H Ly}\alpha$ line
- $\text{H}_2$ CIA line

Graph details:
- $F_\lambda$ (erg cm$^{-2}$ s$^{-1}$ Å$^{-1}$) on the y-axis
- $\lambda$ (Å) on the x-axis
- Two model curves: $T_{\text{eff}}=3800K$, $\log g=7.0$, pure-He in blue, $T_{\text{eff}}=3950K$, $\log g=7.0$, pure H in red

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Pure-H models are reliable. Do we understand He-rich atm. cool WDs?

- The ionization fraction of dense He is highly uncertain, but definitely higher than that of the ideal gas (*our model* (Kowalski et al, PRB, 2007, 76, 075112) consistent with recent data of Celliers et al., 2010, PRL, 104, 184503)

**Experimental data on dense H/He needed!**

Questions/problems addressed by *ab initio* calculations:

- Is negative hydrogen ion stable in fluid helium?
- Properties of $C_2$ in dense He – what is the origin of “peculiar” cool DQ stars?
H⁻ in dense helium

Methodology
- DFT (PBE, uspp) + Car-Parrinello quantum molecular dynamics

Conclusions
- H⁻ is stable in dense He – it doesn't ionize up to density of 2g/cm³.
- The ionization energy of negative hydrogen ion increases with density up to ~2g/cm³.
C$_2$ in dense helium – origin of “peculiar” DQs

- DQ stars disappear at T$_{\text{eff}}$ $\sim$ 6000K, “peculiar” DQs were detected at lower T$_{\text{eff}}$
- Initially assigned to a new molecular species: C$_2$H (Schmidt et al., 1995, ApJ)
- Shifts not due to a different species and not constant (Hall & Maxwell 2008)
C$_2$ in dense helium (in DQs)

Photospheric density increases with decreasing the effective temperature; DQ->DQp transition should be a density effect!

Graphs showing:
- Log C/He vs. $T_{\text{eff}}$ (K) for different densities.
- $\Delta T_e$ (eV) vs. density ($\rho$ (g/cm$^3$)).

$T_e = 2.49$ eV

$\omega_e$ is not affected up to density of 0.5 g/cm$^3$
Understanding the spectra of “peculiar” DQs

LHS 290
“peculiar” DQ

$T_{\text{eff}} = 5800 \text{K}$

Kilic et al., 2010: J1442+4013 (DQp), $T_{\text{eff}} = 5737 \text{K}$, H/He = 2.09 $10^{-3}$
Cool DQ stars

Conclusions
• In cool DQ stars the Swan bands should be blueward shifted
• LHS 290: without H, the modeled density is an order of magnitude larger than the one needed to produce the observed shifts

Solution
• pollution by hydrogen
• incomplete knowledge of helium-rich medium

Kowalski, 2010, submitted
Summary

• Our H-rich models perform very well (good fits including fits to SEDs of the coolest WDs (Halo members) and WD in binary system with Pulsar).

• Helium-rich atmosphere white dwarfs should be explained.

• Ab initio methods valuable for investigation.

• Investigation of H⁻ & C₂ in dense helium: H⁻ is stable (up to 4g/cc) & Swan bands should be shifted to the blue; “Peculiar” DQ WDs most probably DQs showing pressure shifted carbon bands.
Acknowledgments

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