"*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)*

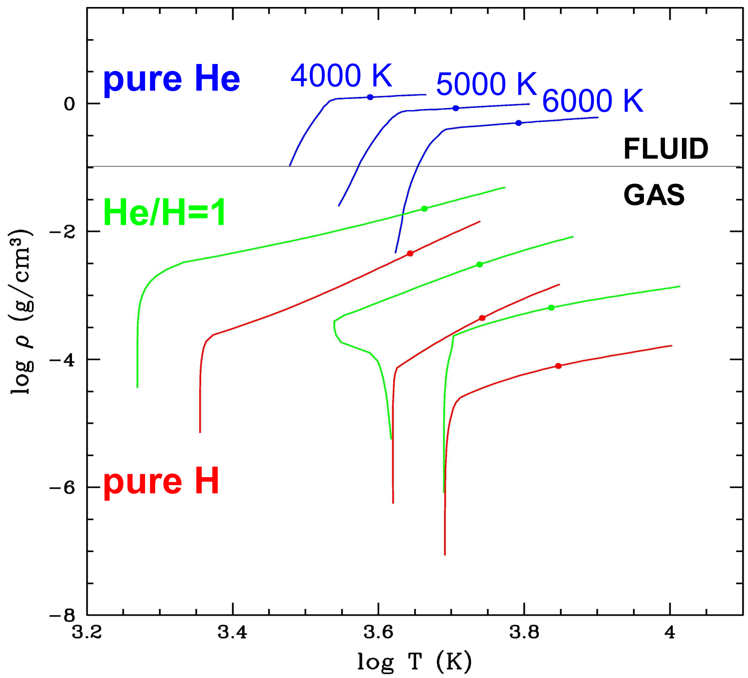
Atmospheres of cool WDs

Important

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

Problematic

- H-lines detectable down to T_{eff}~5000K
- 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)*

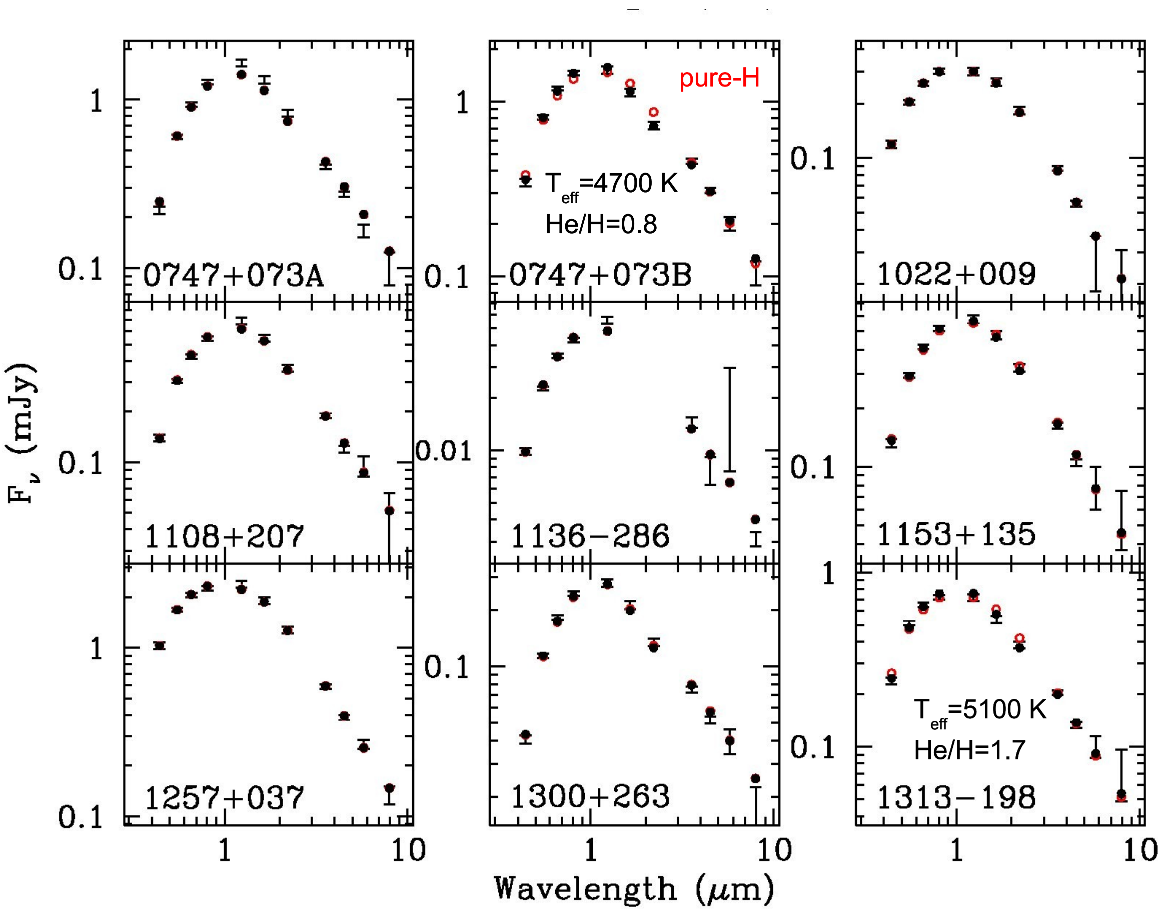
Ab initio models for:

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

Our improvements

Current state	Our improvements
Radiative transfer for planar non-refractive atmosphere	**Radiative Transfer Equation** in a refractive medium
Currently, the following species are included: H_2 H H^+ H_2^+ H_3^+ H^- He He_2^+ He^+ HeH^+ e^- , but chemistry is that of ideal gas *(except ionization equilibrium of He)*	**The non-ideal chemical equilibrium abundances of species: H, H_2, H^-, He, He^+, He_2^+, e^-**
Dilute gas photo absorption **cross-sections** and **chemistry**	**A revision of the most important sources of opacities in helium-rich WD atmospheres: He^- ff, H^- bf**
Flux excess in the model spectra of hydrogen atmosphere white dwarfs	**Found the missing absorption mechanism at short wavelengths (Lyα)**
Unknown nature of "peculiar" DQs	**Density induced spectral distortion of C_2 bands**

Performance: fits to the SEDs of cool WDs



Majority of cool DC stars have hydrogen rich atmospheres?!

Kilic, Kowalski et al. ApJ 696, 2094 (2009)

Performance: WDs Halo candidates

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

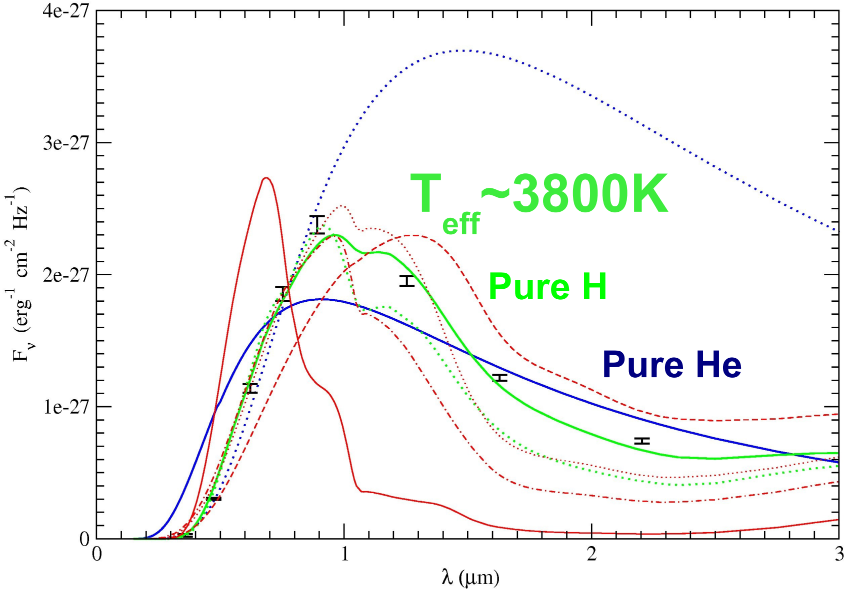
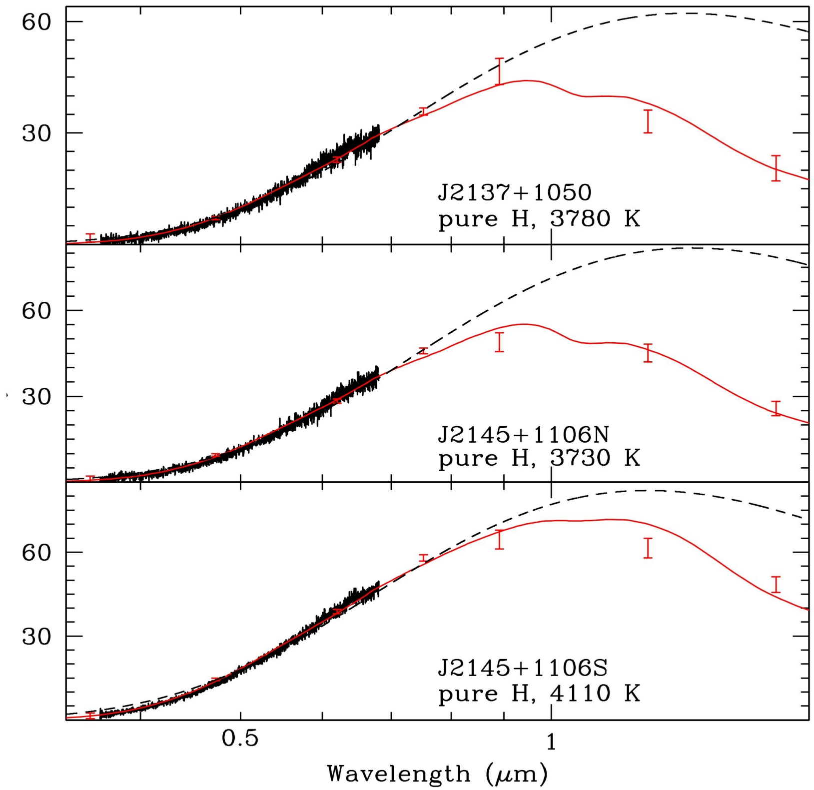


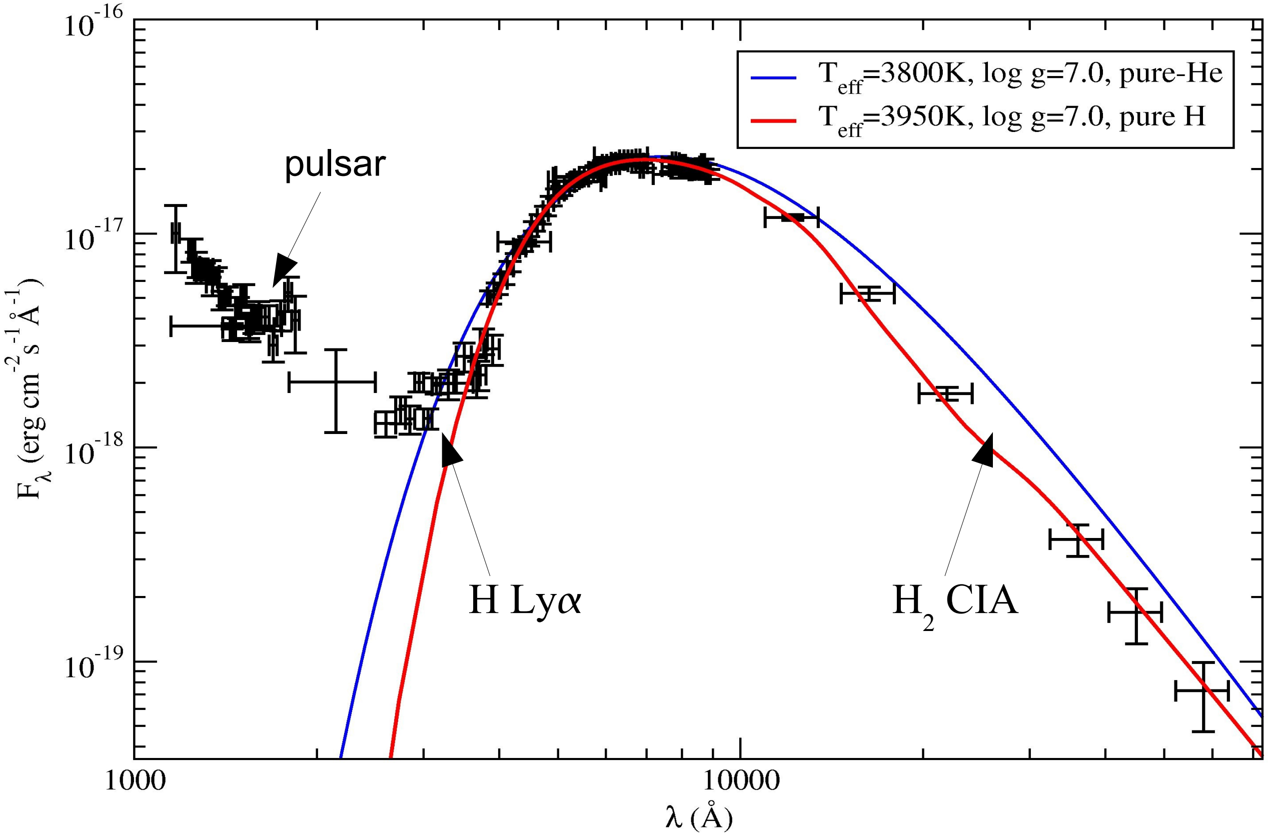
FIG. 5.— Synthetic spectra of pure H, pure He and mixed H/He models, all assuming $\log g = 8$. Fits to all data yield $T_{\rm eff}$=3830 K for pure H (solid green) and $T_{\rm eff}$=5381 K for pure He (solid blue). Fits to optical data only yield $T_{\rm eff}$=3450 K for pure H (dotted green) and $T_{\rm eff}$=3360 K for pure He (dotted blue). Helium-dominated models with $T_{\rm eff}$=3500 K are shown by the red lines, with hydrogen contents as follows: log H/He = −3 (solid), −4 (dash-dotted), −5 (dotted) and −5.5 (dashed).

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



WD in a binary system with a pulsar

Binary system: pulsar PSR J0437-4715 + WD



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?

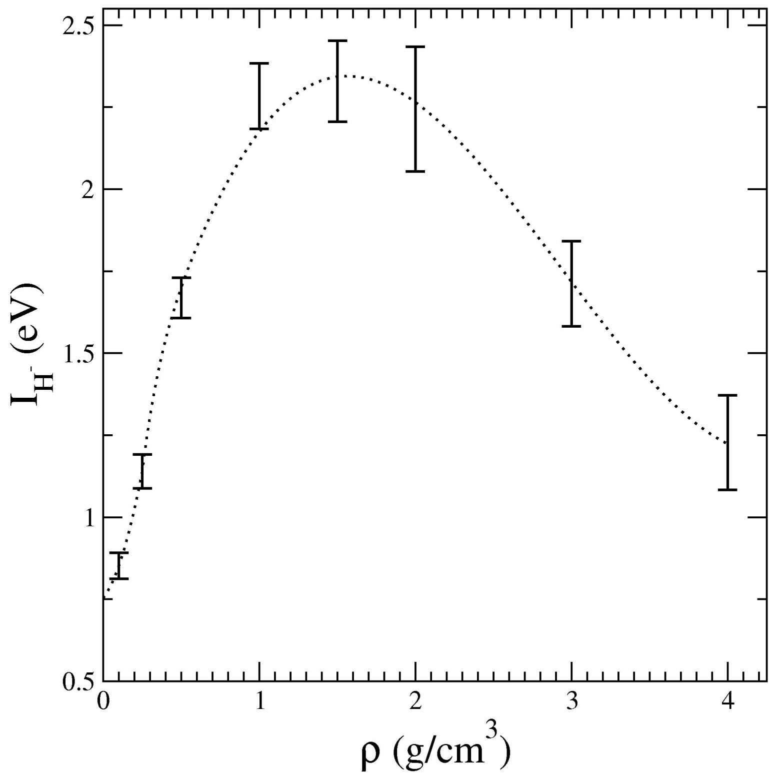
H^- in dense helium

Methodology

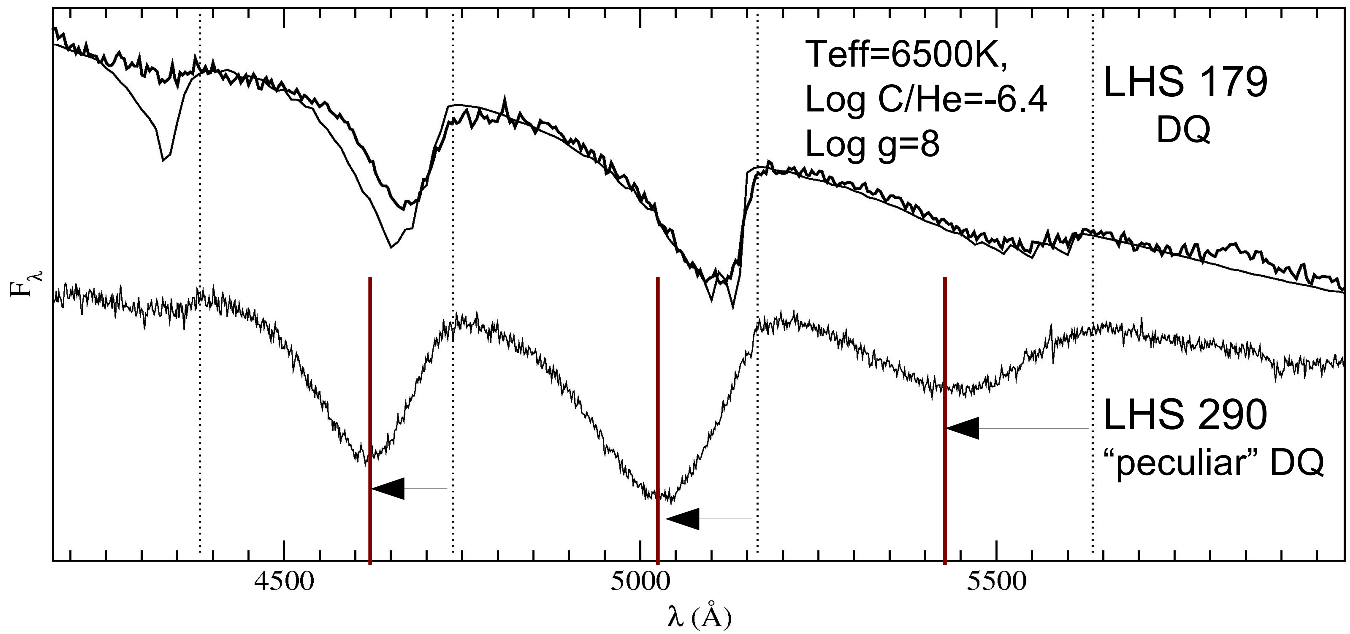
- DFT (PBE, uspp) + Car-Parrinello quantum molecular dynamics

Conclusions

- H^- is stable in dense He – it doesn't ionize up to density of 2g/cm^3.
- The ionization energy of negative hydrogen ion increases with density up to ~2g/cm^3.

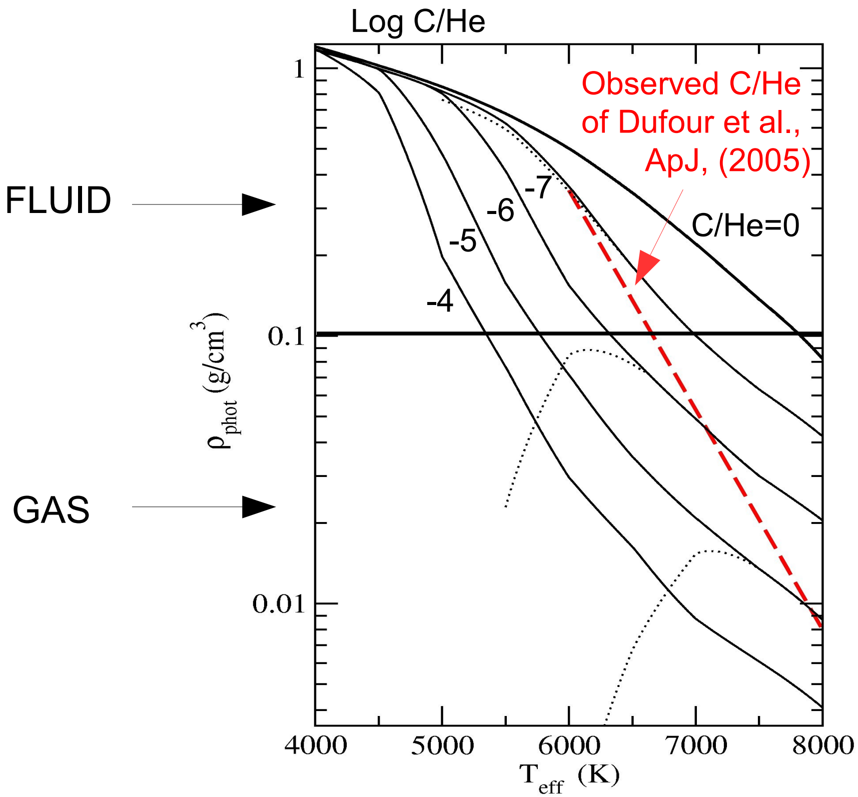


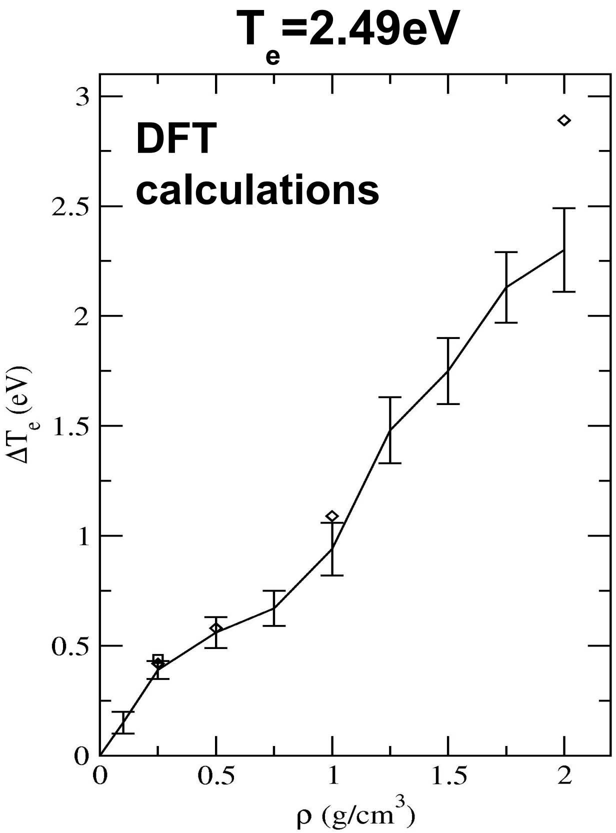
C_2 in dense helium – origin of " peculiar" DQs



- DQ stars disappear at T_{eff}~6000K, "peculiar" DQs were detected at lower T_{eff}
- Initially assigned to a new molecular species: C_2H *(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)

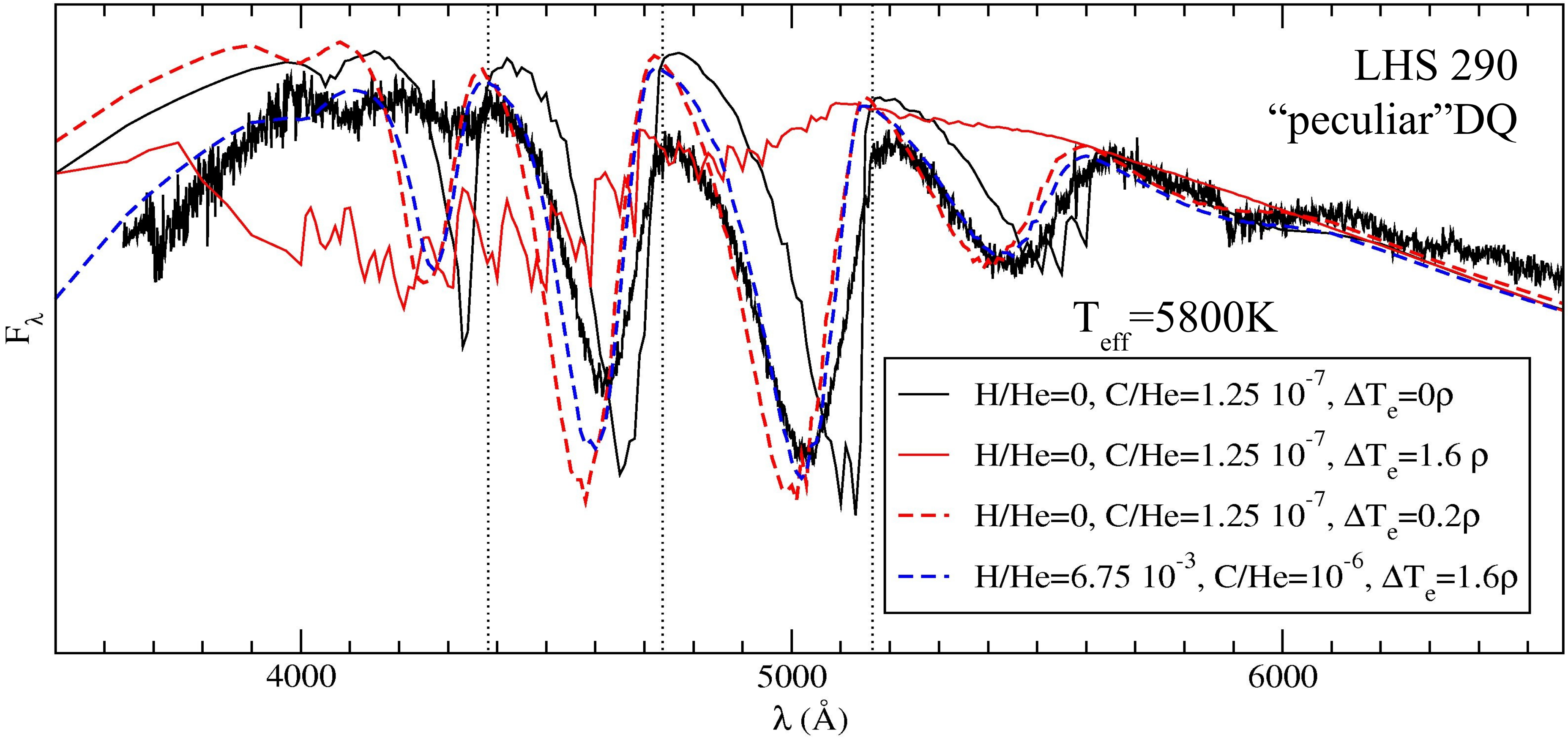




ω_e is not affected up to density of 0.5 g/cm^3

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

Understanding the spectra of “peculiar” DQs



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

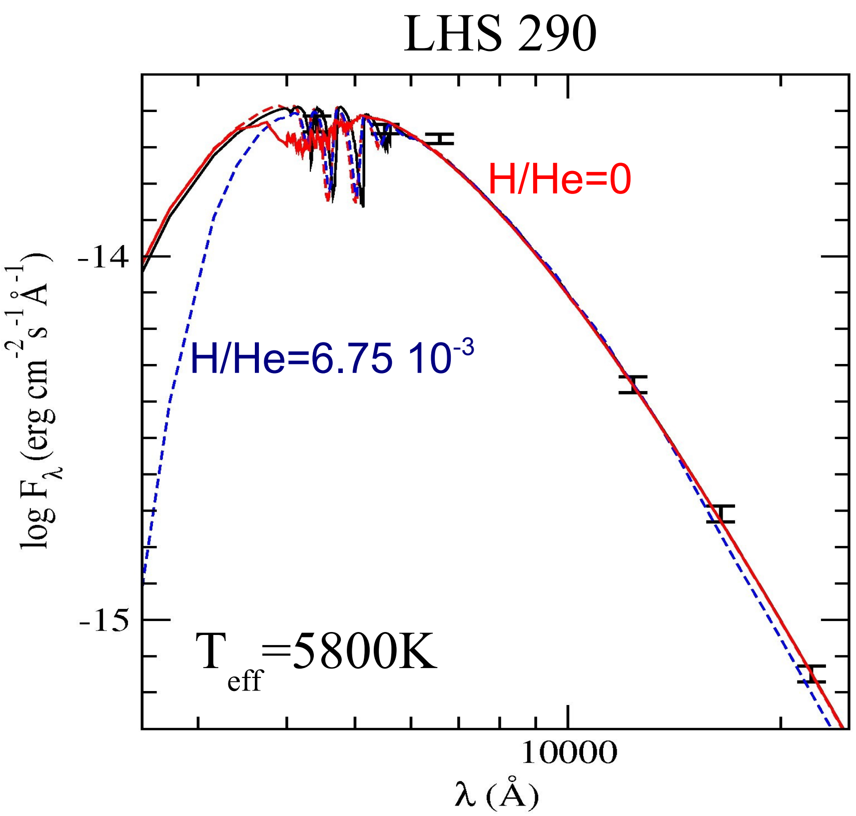
Cool DQ stars

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^- & C_2 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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Thanks for your attention!