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| Name: | Aodong Liu |
| Date: | 02/08/2022 |

**INDIVIDUAL DEVELOPMENT PLAN (ADVISEE)**

The IDP is a tool to help you set long-term goals and track your progress in graduate school. Use this form every year after your first year and review annually with your advisor. After discussing with your advisor, you will both sign the last page and maintain a copy for your records. This document is not collected by the department. You will be asked to affirm that you have completed your IDP each year, and 2nd year students will review their completed IDP (both advisee and advisor sections) with their 2nd year exam committee.

1. List any publications, presentations, seminars, awards, and/or any other notable benchmarks you have achieved.

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| * Excellence in Chemistry Graduate Fellowship Award * Paper tentatively titled “Simultaneous Optimization of Electronic and Nuclear Wavefunctions under the Nuclear-Electronic Orbital Framework” in preparation |

1. Use the relevant sections of the timeline below to describe your goals and to outline how you will achieve them. Have your goals or plans changed since the last update meeting?

**Proposed Project Timeline**

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| **Time Scale** | **Activities to Attain Goals** |
| *This week* | * Bugfixing my code so that it works with the most recent version of development version of Gaussian software * Running more calculations to benchmark the performance of my newly implemented algorithm * Doing data analysis on the Cholesky Decomposition (CD) projects |
| *This month* | * Finish writing up the paper on my nuclear-electronic orbital (NEO) optimization project * Finish cleaning up the code in Gaussian * Make progress doing data analysis for CD project |
| *Six months* | * Implement density functional theory (DFT) for my new algorithm. Then move on to developing NEO-dynamics in gaussian * Finish CD project * Application projects with IDream |
| *One year*  *(next meeting)* | * Do good science and have several publications * Be more knowledgeable and more proficient in programming * Learn more about quantum computing and hopefully do related projects |
| *Long-term*  *(best guess)* | * Become an expert in non-adiabatic electronic dynamics * Pursuit jobs in industry |

1. Summarize your scientific progress since the last update meeting. What key benchmarks of progress have you achieved in your project?

* (Almost) finished my NEO-DIIS project, in the process of wrapping it up
* Learning about RT-TDDFT and Ehrenfest dynamics
* Learning the language of Fortran and how to code in Gaussian
* Doing benchmark on Cholesky Decomposition project (with algorithm optimized for general contracted basis sets), and have obtained good preliminary results

1. What do you perceive as your strengths and why? Consider your ability to understand the current state of your field, formulate open research questions, plan research tasks, make day-to-day and long-term research progress, interpret results, consider alternative models, maintain a detailed lab notebook, communicate your work in written and oral formats, and mentor other researchers.

My strength is that I tried to learn as much as I can on the job. Every time I learn some knowledge, I try to dig deeper and try to truly grasp it. I have a good habit of writing scripts with lots of comments so that I will know what to do the next time.

Also, running jobs can take quite a long time. I try to make the most use of my time by reading related literature or doing derivations.

Moreover, I was taught that I must truly know the theory before attempting to implement it in the program. Thus, for every electronic structure theory/method I’ve learned, I have my own derivations with excessive details. This allows me to easily code things up and consolidate my understanding of the science.

1. What area(s) do you feel need the most improvement and why?

* I feel like my time management is not very great. I would set out goals of the day but easily get distracted by other things. I need to learn to focus on the priority and make better use of my time
* I know too little about the post HF calculations. So far I’ve only been working with HF/TDF, and propagation in the time domain. I would really like to learn more about the corrections to HF
* I also need to learn more about tools that can boost my efficiency. Only recently did I learn how to use git, and it was very beneficial. I’ve improved my skills on script writing to simply my tasks but I can improve more as time goes on
* I still don’t think I have a very solid mathematical background, which sometimes makes the derivation harder to see. I would like to take more math courses if possible in the future, the same for the computer architecture and other important fields.

1. What obstacles do you believe you might encounter while pursuing your goals (related to e.g. background knowledge, training, outside responsibilities, and/or health issues)?

* As mentioned above, I have to learn lots of things on the job (math, CS, HPC, coding)
* No health issue for me
* No TA responsibility

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1. Describe any professional opportunities (such as conferences, technical learning, teaching or mentoring experience, fellowships, or participation in courses, workshops, or training programs) that you think will benefit you in the next year.

* If possible, I would like to go to ESQC (European summer school of quantum chemistry)
* Any summer school experiences would be beneficial
* Will be taking more quantum computing class

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1. Do you feel that you are getting what you need from your advisor as a mentor? Is there one thing your advisor could focus on in the coming year to help you better reach your goals?

Yes I do feel I’m getting what I need. We have many subgroup meetings to talk about my research progress

1. Do you have any suggestions for improving the operation of the research group?

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| No. |

1. Describe any other graduate school or career development topics you would like to discuss with your PI regarding the attainment of your long-term goals.

* I actually recently talked with my PI about career development. He gives me suggestions on what classes that will benefit me, and what projects might interest me.

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1. List any classes you plan to take in the next academic year, including any classes outside of the Chemistry department.

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| * Quantum Computing in the spring quarter * Maybe more numerical analysis classes |

1. Have you experienced any disparate treatment based on any component of your identity (race, ethnicity, gender, sexual orientation, etc…)? If you are not comfortable discussing this issue with your advisor, please consider reaching out to others for support including the Graduate Program Coordinator (Christine Gormley), any faculty member on the PhD Training & Mentoring Committee, a union ASE steward, UW SafeCampus, and/or the UW Ombud office.

No.

**MENTORING PLAN (ADVISOR)**

Advisee completes their section first, then advisor completes this section.

1. Are your advisee’s proposed goals and timeline realistic? Is your advisee progressing towards these goals at a sufficient rate? What strategies do you recommend your advisee use to reach these goals?

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| Yes, Aodong’s proposed goals and timeline are realistic. He is progressing nicely towards these goals. He is already doing all the right things in order to reach these goals. |

1. What are your expectations of your advisee for this next year (e.g. commitment of time/effort, scheduling, and/or benchmarks of progress)?

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| I hope Aodong will finish developing the simultaneous optimization algorithm for NEO-SCF and write/publish two research papers based on his current results. |

1. Describe any professional opportunities (such as conferences, technical learning, teaching, or participation in courses) that you think will benefit your advisee within the next year. What resources or people (e.g. organizations, campus services, or collaborators) do you suggest your advisee contact?

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| If the European Summerschool in Quantum Chemistry reopens, I hope Aodong will attend it. Since Aodong will continue the collaboration with Prof. Hammes-Schiffer at Yale, regular meetings with collaborators are needed. |

1. Describe any other graduate school or career development topics you would like to discuss with your advisee regarding attainment of long-term goals.

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| Internships at national labs can be helpful. |

Aodong Liu 02/08/2022

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|  |  |  |  | 1/31/2022 |
| Date of next meeting |  | Advisee Signature Date |  | Advisor Signature Date |

*Advisee keeps original document and delivers a copy to the advisor. Electronic versions OK.*