# Capability profile

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Capability profile is defined as capacity to perform tasks in a given role. It consists of 2 components.

- i) Core function main function of a given role
- ii) Competency related competencies of a profile

There are 5 levels of each discipline as follows.

- 1. **Apprentice** Have limited set of skills. Able to work on guided projects or narrow specific tasks. Supervision is needed for brand-new or complex tasks.
- 2. **Practitioner** Have basic set of skills covering the majority of aspects. Able to work on specific tasks. Recommendation is needed for complex tasks.
- 3. **Competent** Able to apply set of skill to solve real-world problem. Able to solve common problems independently.
- 4. **Proficient** Able to lead a project for solving real-world problems. Able to solve unseen problems with some advice.
- 5. **Expert** Able to lead a team to conduct a research or development project. Able to solve unseen problems and create new research protocols.

#### Disclaimer

This competency and capability profile framework does not cover the diversity of background knowledge in research domain. They are packed in *D1 Scientific background knowledge, methodology, process, and tools*. The diversities are in *A high performance computing* and *B computing competency*. The competency of *E Soft skills* is not covered in this version.

# Roles

HPC AI specialist apprentice	3
HPC AI specialist practitioner	
HPC AI specialist competent	5
HPC computational chemistry specialist apprentice	6
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HPC computational chemistry specialist competent	8

# HPC AI specialist apprentice

### Computational core function

- Able to utilize a node of HPC for running AI workload
- Able to prepare a Python environment by following a guideline
- Able to work in batch and offline mode which is a common HPC environment

### Research core function

- Basic knowledge of related topics
- Communicate finding results

- A1 remember
- A2 remember
- B1 apply
- B2 understand
- B3 remember
- B4 apply
- B5 remember
- C1 understand
- D1 understand
- D2 remember
- D3 apply

# HPC AI specialist practitioner

### Computational core function

- Able to utilize HPC for running AI workload using multinode
- Able to prepare a Python environment by adapting from a guideline
- Able to set relevant environment variables efficiently by following guidelines
- Able to work in batch and offline mode which is a common HPC environment

### Research core function

- Basic knowledge of related topics
- Able to find relevant articles, publications, or repositories
- Communicate finding results

- A1 understand
- A2 apply
- A3 understand
- B1 apply
- B2 apply
- B3 understand
- B4 apply
- B5 apply
- C1 understand
- D1 understand
- D2 understand
- D3 apply

## HPC AI specialist competent

#### Computational core function

- Able to utilize HPC for running AI workload using multinode efficiently
- Able to write guidelines to prepare a Python environment for specific environment
- Able to set relevant environment variables efficiently by applying knowledge from guidelines
- Able to work in batch and offline mode which is a common HPC environment

### Research core function

- Basic knowledge of related topics
- Able to find and describe relevant articles, publications, or repositories
- Share ideas and efficiently communicate finding results

- A1 apply
- A2 analyze
- A3 apply
- B1 evaluate
- B2 analyze
- B3 understand
- B4 analyze
- B5 analyze
- C1 apply
- D1 apply
- D2 apply
- D3 apply

# HPC computational chemistry specialist apprentice

## Computational core function

- Able to utilize HPC for performing given tasks according to the instructions strictly
- Able to work in batch and offline mode which is a common HPC environment

### Research core function

- Basic knowledge of related topics
- Communicate finding results

- A1 remember
- A2 remember
- B1 apply
- B3 remember
- B4 understand
- C1 remember
- D1 understand
- D2 remember
- D3 apply

# HPC computational chemistry specialist practitioner

### Computational core function

- Able to utilize HPC for performing given tasks by applying knowledge from guidelines
- Able to set relevant environment variables efficiently by following guidelines
- Able to work in batch and offline mode which is a common HPC environment

#### Research core function

- Basic knowledge of related topics
- Able to find and describe relevant articles, publications, or repositories
- Communicate finding results

- A1 understand
- A2 apply
- A3 understand
- B1 apply
- B3 understand
- B4 apply
- B5 apply
- C1 understand
- D1 understand
- D2 understand
- D3 apply

## HPC computational chemistry specialist competent

# Computational core function

- Able to utilize HPC for performing a given task from a guideline efficiently
- Able to set relevant environment variables efficiently by applying knowledge from guidelines
- Able to prepare software and related environments by following guidelines
- Able to work in batch and offline mode which is a common HPC environment

### Research core function

- Basic knowledge of related topics
- Able to find and describe relevant articles, publications, or repositories
- Share ideas and efficiently communicate finding results

- A1 apply
- A2 analyze
- A3 apply
- B1 evaluate
- B2 apply
- B3 apply
- B4 analyze
- B5 analyze
- C1 apply
- D1 apply
- D2 apply
- D3 apply