

|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------|-------------------------------------------------------------------------|--------------------------------------------------------------------|---------------------------------------------------------------------------------------------------|-----------|-----------------------------------------|--|
| 茨城工業高等専門学校                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                                                       | 開講年度                                                                    | 令和03年度 (2021年度)                                                    |                                                                                                   | 授業科目      | Quantum Chemistry                       |  |
| 科目基礎情報                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                       |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
| 科目番号                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 0132                                                                  |                                                                         |                                                                    | 科目区分                                                                                              | 専門 / 選択   |                                         |  |
| 授業形態                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 講義                                                                    |                                                                         |                                                                    | 単位の種別と単位数                                                                                         | 学修単位II: 2 |                                         |  |
| 開設学科                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | 国際創造工学科 電気・電子系                                                        |                                                                         |                                                                    | 対象学年                                                                                              | 5         |                                         |  |
| 開設期                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | 後期                                                                    |                                                                         |                                                                    | 週時間数                                                                                              | 後期:2      |                                         |  |
| 教科書/教材                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                | 1) Quantum Mechanics for Chemists, by David Howard.                   |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
| 担当教員                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  | アッバス アルシハビ                                                            |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
| 到達目標                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                       |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
| 1) understand the difference between classical and quantum mechanics.<br>2) understand the idea of wave function.<br>3) understand the uncertainty relations.<br>4) solve Schroedinger equation for simple potentials.<br>5) understand the Schroedinger theory application to Hydrogen atom.<br>eigenvalue problems for energy, momentum, angular momentum and central potentials explain the idea of spin.<br>6) solve the<br>7) understand the Schroedinger theory application to many-electron atoms.<br>the Orbital Molecular Theory.<br>8) become introduced to |                                                                       |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
| ルーブリック                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                                                       |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | Ideal Level                                                           | Standard Level                                                          | Minimum achievement level standard (Pass)                          | Unacceptable Level                                                                                |           |                                         |  |
| Understand the principles of quantum mechanics                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        | Treat wave functions in linear algebra.                               | Understand the atomic wave function.                                    | Know the difference between classical and quantum mechanics        | Does not understand the postulates of quantum mechanics.                                          |           |                                         |  |
| Understand the Schroedinger Theory of Quantum Mechanics                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               | Define the equation for the well, and barrier potential applications. | Define the equation, and define components.                             | Understand the component of the Schroedinger equation.             | Does not understand the Shroedinger equation components.                                          |           |                                         |  |
| Understand the Schroedinger application to the Hydrogen atom.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         | Define the equation and calculate the eigen values.                   | Calculate the eigen values from the Schrodinger Equation.               | Define the Hydrogen atom eigen values in the Schrodinger equation. | Does not understand the eigen values in the Schroedinger equation.                                |           |                                         |  |
| Understand the Molecular Orbtal Theory application.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | Can write the electronic configuration of the molecular orbital.      | Make a Molecular Orbital energy level diagram of an elemental molecule. | Understand the bonding mechanism in the Molecular Orbital Theory.  | Does not understand the Schroedinger application to the multi-electron atom.                      |           |                                         |  |
| 学科の到達目標項目との関係                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |                                                                       |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
| 学習・教育到達度目標 (A)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                                                       |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
| 教育方法等                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |                                                                       |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
| 概要                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | Lecturing: Slide show, blackboard explanation.                        |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
| 授業の進め方・方法                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             | Tutorial: solving backboard questions, homework                       |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
| 注意点                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   | This class is held in English.                                        |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
| 授業の属性・履修上の区分                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |                                                                       |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
| <input type="checkbox"/> アクティブラーニング                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |                                                                       | <input type="checkbox"/> ICT 利用                                         |                                                                    | <input type="checkbox"/> 遠隔授業対応                                                                   |           | <input type="checkbox"/> 実務経験のある教員による授業 |  |
| 授業計画                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                       |                                                                         |                                                                    |                                                                                                   |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 週                                                                       | 授業内容                                                               | 週ごとの到達目標                                                                                          |           |                                         |  |
| 後期                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    | 3rdQ                                                                  | 1週                                                                      | Principles of quantum mechanics; revision                          | Understand the principles,                                                                        |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 2週                                                                      | Postulates of Quantum mechanics                                    | Understand the wave function.                                                                     |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 3週                                                                      | Postulates of Quantum mechanics                                    | Undertsnad linear operators, Hamiltonian.                                                         |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 4週                                                                      | Schroedinger theory of quantum mechanics 1                         | Undesrand Born`s Interpretation, Infinite square well potential                                   |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 5週                                                                      | Schroedinger theory of quantum mechanics 2                         | Understand The Time-Independent Schroedinger Equation                                             |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 6週                                                                      | Schroedinger theory of quantum mechanics 3                         | Understand the solutions to the Time-Independent Schroedinger Equation; zero and step potentials. |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 7週                                                                      | Midterm Exam                                                       |                                                                                                   |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 8週                                                                      | Schroedinger theory of quantum mechanics 4                         | Understand Zero potential and step potentials.                                                    |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | 4thQ                                                                  | 9週                                                                      | Schroedinger theory of quantum mechanics 5                         | Understand barrier potential and harmonic oscillator potential.                                   |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 10週                                                                     | The Hydrogen atom 1                                                | Understand the application of Shroedinger`s equation to the Hydrogen atom.                        |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 11週                                                                     | The Hydeogen atom 2                                                | Solve the Shroedinger`s equation for the Hydrogen atom.                                           |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 12週                                                                     | Multi-electron atom                                                | Understand the application of Shroedinger`s equation to the multielectron atoms.                  |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 13週                                                                     | Molecular Orbital Theory                                           | Become introduced to Hartree Fock approximation                                                   |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 14週                                                                     | Molecular Orbital Theory                                           | Become introduced to molecular orbital theory, Hydrogen molecule bonding                          |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 15週                                                                     | Final Exam                                                         |                                                                                                   |           |                                         |  |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |                                                                       | 16週                                                                     | Review                                                             | Review                                                                                            |           |                                         |  |
| 評価割合                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                                                       |                                                                         |                                                                    |                                                                                                   |           |                                         |  |

|                         | Presentation | Homework/Report | Mutual Evaluations between students | Behavior | Portfolio | Quiz | 合計  |
|-------------------------|--------------|-----------------|-------------------------------------|----------|-----------|------|-----|
| 総合評価割合                  | 0            | 45              | 0                                   | 0        | 0         | 55   | 100 |
| Basic Proficiency       | 0            | 15              | 0                                   | 0        | 0         | 15   | 30  |
| Specialized Proficiency | 0            | 15              | 0                                   | 0        | 0         | 25   | 40  |
| Cross Area Proficiency  | 0            | 15              | 0                                   | 0        | 0         | 15   | 30  |