

Department of Chemistry and Centre for research

Q.No: Report of - Five Day Online Faculty Enrichment Programme On Quantum Mechanics

Title of the Programme : Five Day Online Faculty Enrichment Programme On Quantum Mechanics

Date : 18/01/2021 - 22/01/2021

Venue : Google Meet

No: of Beneficiaries/ Participants : 67

Beneficiary type : Researchers and Teachers

Activity Description (100 - 200 words) Five Day Online Faculty Enrichment Programme on Quantum Mechanics from 18-01-2021 to 22-01-2021 was organized by the Teresian Teaching Learning Centre and the Department of Chemistry and Centre for Research, St. Teresa's College in collaboration with Chemical Research Society of India Local Chapter with the support of all Chemistry teachers in India. The event was organized through Google Meet and started everyday at 7 pm and ended at 8:30 pm. The resource person was Dr. R.S. Swathi, Associate Professor, School of Chemistry, IISER-Thiruvananthapuram. On demand from the participants, the FEP was extended to one more day to 23-01-2021.

67 teachers participated in the enrichment program which covered the following topics:

1. Historical background-Ideas that led to the birth of quantum mechanics.
2. Postulates of quantum mechanics, mathematical foundations
3. Particle in a box, quantum tunneling
4. Electronic structure of He
5. Molecular orbital treatment
6. Modelling conjugated systems

The topics were selected after conducting a needs assessment survey among the participants.

The recordings of the five day session is available in the following links:

Day 1: The Story of the Birth of Quantum Mechanics:

https://drive.google.com/file/d/1_jmCBVmXhT6QoO_RNu-8xBotBAYFY0GX/view?usp=sharing

Day 2: Mathematical Foundations of Quantum Mechanics:

https://drive.google.com/file/d/1CvAFpqBpmGSNq_eQilfah8BXZEH7joQt/view?usp=sharing

Day 3: Manifestations of Tunneling:

https://drive.google.com/file/d/1VH_OWmleefTtwXcM_eWrV_LZ1g8Uz2W8/view?usp=sharing

Day 4: Electronic Structure of Helium

https://drive.google.com/file/d/12SJD45y3Y3ipw0jul5_KQV8rpD27I8YS/view?usp=sharing

Day 5: Molecular Orbital Treatment of Molecular Hydrogen:

https://drive.google.com/file/d/1SeaOLY3vgB0_cIGR8g3asVltAg2Mp_eQ/view?usp=sharing

Day 6: Modelling conjugated systems and hybridization:

<https://drive.google.com/file/d/1PPSWPe6hjsNNaktiaaAmpRz9vXsUDC0u/view?usp=sharing>

Outcome of the activity : The participants were able to clarify their doubts on various aspects of quantum mechanics and understand the key concepts.

Brochure :



**FACULTY ENRICHMENT PROGRAM
ON
QUANTUM MECHANICS**
18-22 January, 2021 | 7-8.30 pm

RESOURCE PERSON
Dr. R.S. Swathi
Associate Professor
School of Chemistry
IISER-TVM

ORGANISED BY
Teresian Teaching Learning Centre and
Department of Chemistry and Centre for Research
St. Teresa's College (Autonomous), Ernakulam
Accredited with NAACA⁺ and ranked 47th in NIRF

IN ASSOCIATION WITH
Chemical Research Society of India (CRSI)

COORDINATORS

Dr. Saritha Chandran A (9048799993), Assistant Professor in Chemistry and Coordinator - Teresian T.L.C., St. Teresa's College	Dr. Elizabeth Kuruvilla (6282385804), Assistant Professor in Chemistry, St. Teresa's College	Dr. Mahesh Hariharan, Professor, School of Chemistry, IISER-TVM & Convener, Local Chapter, CRSI
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One or two photos (Geotagged):

FEP-Quantum Mechanics (2021-01-18 at 05:30 GMT-8) Open with

(16)

The ground state electronic energy for H-atom is
 $E_1 = -13.6 \text{ eV}$.

The ionization potential is 13.6 eV.

The radius of the first Bohr orbit is
 $r = \frac{4\pi\epsilon_0 \hbar^2}{m e^2} = 0.529 \text{ \AA}$.

Interpretation of the quantization condn:
 Only stationary orbits are those that are

48:37 / 3:30:10

FEP-Quantum Mechanics (2021-01-19 at 05:28 GMT-8) Open with

Thought experiments with double slits - Feynmann:

Double slit exp't with bullets:

Watch in Picture-in-Picture

3:48 / 1:29:43

Region II:

$$\frac{-\hbar^2}{2m} \frac{d^2 \psi_{II}}{dx^2} + V \psi_{II} = E \psi_{II}$$

$V = 0$ in region II.

$$\therefore \frac{d^2 \psi_{II}}{dx^2} = -\frac{2mE}{\hbar^2} \psi_{II} = -k^2 \psi_{II}$$

16:40 / 1:31:15

FEP-Quantum Mechanics (2021-01-21 at 05:32 GMT-8) Open with

This is a free particle Hamiltonian:
 $\therefore E_1 = \frac{\hbar^2 k^2}{2M}$; $\psi_1(\vec{R}) = e^{i\vec{k}\cdot\vec{R}}$

$\left[\frac{-\hbar^2}{2\mu} \nabla_{\vec{r}}^2 - \frac{Ze^2}{4\pi\epsilon_0 r} \right] \psi_2(\vec{r}) = E_2 \psi_2(\vec{r}) \rightarrow$ describes the internal motion

$E_2 = -\frac{13.6 Z^2}{n^2} \text{ eV}$; $\psi_2(\vec{r}) = R_{nl}(r) Y_l^{m_l}(\theta, \phi)$
 Radial wave fn Spherical Harmonic

The Schrödinger eqn for the centre of mass coordinate describes the translational motion of the centre of mass of the atom. This leads to a continuum of energy

Unmute (m) 7:03 / 1:31:20

Watch in Picture-in-Picture

$(H_{11} - E S_{11})(H_{22} - E S_{22}) - (H_{12} - E S_{12})(H_{21} - E S_{21}) = 0$

$H_{11} = H_{22} = \alpha$ (say).

$H_{21} = H_{12} = \beta$ (say).

$S_{11} = S_{22} = 1$; $S_{12} = S_{21} = S$ (say).

$\begin{vmatrix} \alpha - E & \beta - ES \\ \beta - ES & \alpha - E \end{vmatrix} = 0$

Play (k) 9:01 / 1:22:31

Watch in Picture-in-Picture