

# Curriculum Vitae

## Anila Sebastian

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### Educational Qualifications:

- **2022** - Ph. D. in Science under the faculty of Chemical sciences from the Academy of Scientific and Innovative Research (AcSIR) at the CSIR - National Institute For Interdisciplinary Science and Technology (NIIST), Thiruvananthapuram (Kerala, India).
- **2016** - M. Sc. Chemistry from Mahatma Gandhi University, Kottayam (Kerala, India)
- **2014** - B. Sc. Chemistry from Mahatma Gandhi University, Kottayam (Kerala, India)

### Grants and Awards:

- CSIR-UGC JRF December 2016 - All India rank 35.
- GATE 2017 - All India rank 1556.
- Kerala State Higher Education Council Scholarship, integrated five-year meritorious scholarship 2011-2016
- Maulana Azad National Scholarship, meritorious scholarship at the higher secondary level, 2009-2011.

### Publications:

1. **Anila, Sebastian**, and Cherumuttathu H. Suresh. "Fulleride-metal  $\eta^5$  sandwich and multi-decker sandwich complexes: A DFT prediction." *Journal of Computational Chemistry*, 2023, 44, 199-208.
2. **Anila, Sebastian**, and Cherumuttathu H. Suresh. "Nitrogen-doped fullerenes for CO<sub>2</sub> capture: a DFT study." *New Journal of Chemistry*, 2023, 47, 3047-3054.
3. Chitranshi, Sangya; Adinarayana, Bellamkonda; Das, Mainak; **Anila, Sebastian**; Suresh, Cherumuttathu; Srinivasan, Alagar. "Rh(I) and Organo-Rh(III) Complexes of meso-Triarylbi(phenyl)corrole." *Inorganic Chemistry*, 2023, 62, 336–341.

4. **Anila, Sebastian**, and Cherumuttathu H. Suresh, “Polyanionic cyano-fullerides for CO<sub>2</sub> capture: A DFT Prediction.” *Physical Chemistry Chemical Physics*, 2022, 24, 22144-22153
5. **Anila, Sebastian**, Cherumuttathu H. Suresh, and Henry F. Schaefer III, “Demarcating noncovalent and covalent bond territories: Imine-CO<sub>2</sub> complexes and cooperative CO<sub>2</sub> capture.” *Journal of Physical Chemistry A*, 2022 126, 4952-4961.
6. **Anila, Sebastian**, and Cherumuttathu H. Suresh. “Imidazolium–fulleride ionic liquids– a DFT prediction.” *Physical Chemistry Chemical Physics*, 2021, 23, 20086-20094. [**HOT ARTICLE**]
7. **Anila, Sebastian**, and Cherumuttathu H. Suresh. “Guanidine as a strong CO<sub>2</sub> adsorbent: a DFT study on cooperative CO<sub>2</sub> adsorption.” *Physical Chemistry Chemical Physics*, 2021, 23, 13662-13671.
8. **Anila, Sebastian**, and Cherumuttathu H. Suresh. “Endo-and exohedral chloro-fulleride as  $\eta^5$  ligands: a DFT study on the first-row transition metal complexes.” *Physical Chemistry Chemical Physics*, 2021, 23, 3646-3655.
9. **Anila, Sebastian**, and Cherumuttathu H. Suresh. “Formation of large clusters of CO<sub>2</sub> around anions: DFT study reveals cooperative CO<sub>2</sub> adsorption.” *Physical Chemistry Chemical Physics*, 2019, 21, 23143-23153.

#### **Book Chapters**

##### 1. Liquid transport through polymer Composites

Ajith James Jose, Jincymol Kappen, Meghana Mary Thomas, Vipin G Krishnan, **Anila Sebastian** in *Transport properties of polymeric membranes*, (Eds.: Thomas, Sabu, et al.), Elsevier, 2017, Chapter 11. (Book chapter)

##### 2. Gas transport through thermoplastics

Ajith James Jose, **Anila Sebastian**, Meghana Mary Thomas, Vipin G Krishnan, Jincymol Kappen in *Transport properties of polymeric membranes*, (Eds.: Thomas, Sabu, et al.), Elsevier, 2017, Chapter 22. (Book chapter)