

Supplementary Information

Potential mediated electrochemical recycling and sensing of cadmium ions in wastes water over ZnO/SA-g-PPy bio-composite

Sandeep Verma^{a&b}, Ashok K. Sharma^{a*} and Saroj K. Shukla^{b*}

^aThin-Film Lab, Department of Chemistry, Deenbandhu Chhotu Ram University of Science and Technology, Murtial-131039, India

^bDepartment of Polymer Science, Bhaskaracharya College of Applied Sciences, University of Delhi, Delhi 110075, India

*Corresponding authors

E-mail addresses: draksharma.chem@dcrustm.org (Ashok K. Sharma), sarojshukla2003@yahoo.co.in (Saroj K. Shukla)

Table S1. Observed physical parameters during polymerizations.

| Composition | Time for the beginning of polymerization (min.) | Completion time for polymerization (min.) | Temperature change of reaction bath (°C) | pH | Yield of reaction (%) |
|--------------|---|---|--|----|-----------------------|
| PPy | 3.5 | 20.0 | 0.5 | 2 | 67 |
| ZnO/SA-g-PPy | 2.0 | 15.0 | 2.0 | 2 | 78 |

Table S2. IR peaks for PPy, Sodium Alginate (SA), SA-g-PPy, and ZnO/SA-g-PPy.

| Sr. No. | SA (cm ⁻¹) | PPy (cm ⁻¹) | SA-g-PPy (cm ⁻¹) | ZnO/SA-g-PPy (cm ⁻¹) | Assigned group |
|---------|------------------------|-------------------------|------------------------------|----------------------------------|--|
| 1. | -- | -- | 793 | 793 | C-H and N-H ring out-of-plane bending |
| 2. | 927 | 906 | 916 | 916 | C-O-H and C-N-H stretching in SA and PPy ring in-plane bending |
| 3. | 1046 | 1043 | 1045 | -- | C-O-C glycosidic linkage of SA And C-N-C linkage in PPy |
| 4. | 1186 | 1187 | 1188 | 1182 | C-C stretching |
| 5. | -- | 1221 | -- | -- | C-H and N-H in-plane deformation vibrations |
| 6. | -- | 1361 | -- | -- | C-N stretching in polypyrrole ring |
| 7. | 1413 | -- | 1410 | 1401-- | O-H and N-H bend vibration |
| 8. | 1556 | 1552 | 1546 | 1557 | Strong hydrogen bonds between the pyrrole N-H groups and the hydroxyl groups and free COO ⁻ group of adjacent SA. |
| 9. | 1637 | 1706, 1723 | 1712 | 1712 weak | Interaction of Zn ²⁺ with polypyrrole and COO ⁻ |
| 10. | 2950 | 3004 | 2804, 2881 | 2835 | C-H sp ³ |

| | | | | | |
|-----|------|------|------|------|-------------|
| 11. | 3430 | 3406 | 3298 | 3644 | N-H and O-H |
|-----|------|------|------|------|-------------|

Table S3. XRD data and structural parameters

| S. No. | Sample | Angle (2θ) | Plane (hkl) | d-value (Å) |
|--------|--------------|------------|-------------|-------------|
| 1. | SA-g-PPy | 25.10° | 110 | 3.55 |
| 2. | ZnO | 31.78° | 100 | 2.41 |
| | | 34.44° | 002 | 2.09 |
| | | 36.22° | 101 | 1.47 |
| | | 47.55° | 102 | 1.90 |
| | | 56.64° | 110 | 1.60 |
| | | 62.91° | 103 | 1.46 |
| | | 66.35° | 200 | 1.40 |
| | | 67.97° | 112 | 1.37 |
| | | 69.18° | 201 | 1.35 |
| | | 17.88° | 110 | 4.96 |
| 3. | ZnO/SA-g-PPy | 23.65° | 110 | 3.85 |
| | | 26.29° | 110 | 3.39 |
| | | 30.57° | 100 | 2.96 |
| | | 32.92° | 100 | 2.25 |
| | | 36.28° | 101 | 1.46 |

Table S4. IR peaks and corresponding intensity of ZnO/SA-g-PPy electrode-based sensor, after sensing and before sensing of Cd²⁺ ions.

| Before Sensing | | After Sensing | |
|-----------------------------------|-----------|-----------------------------------|-----------|
| Peak Position (cm ⁻¹) | Intensity | Peak Position (cm ⁻¹) | Intensity |
| 617 | 37.89 | 617 | 136.89 |
| 1041 | 42.18 | 1116 | 92.84 |
| 1413 | 24.44 | 1398 | 165.38 |
| 1557 | 16.86 | 1384 | 151.24 |
| 1648 | 39.78 | 1619 | 150.58 |
| | | 1713 | 153.87 |