The present Raman spectra result do not show the second Raman broad peak normally observed at 1121 cm-1. Researchers attributed the emergence of such band to surface phonon modes, which usually appear in transverse optical – longitudinal optical phonon gap. In this case, only 1 line at 1030 cm-1 is observed.



Figure s1: Raman spectra for annealed MgO nanoparticles

Figure s2 shows the ATR spectra of MgO nanoparticles synthesized via green chemistry using date pits extracts. The spectra present many absorption bands including 3692, 1428, 2990 and 2922 cm−1 that correspond to OH stretching, H2O adsorption, aliphatic group CH2 asymmetric and symmetric vibration respectively. A prominent peak observed at 884cm-1 is an evidence of synthesize of cubic MgO nanoparticles.



Figure s2: ATR spectra of annealed MgO nanoparticles

Figure s3(a,b) present the diffuse reflectance spectra of synthesized MgO nanoparticles at wavelength range between (a) 200-400 nm and (b) 500-2100 nm. As can been seen, regions I and II show absorption bands at 205 and 276nm identified with excitation of four-fold and three-fold coordinated O2− anions in edges and corners of MgO respectively. Annealed at 700℃ MgO nanoparticles exhibit a higher reflectance values from the UV-Vis to NIR wavelength range.



a



b

Figure s3: Diffuse reflectance spectra of un-annealed, and annealed MgO nanoparticles at wavelength rang of (a) 200-400 nm (b) 500-2100

Figure s4 shows the energy band gap spectra of MgO nanoparticles calculated from the diffuse reflectance spectra via the Kubelka–Munk function.



b

a



c

Figure s4: Band-gap representation of (a) un-annealed, (b) MgO nanoparticles annealed at 500℃, (c) MgO nanoparticles annealed at 700℃.

Figure s5 shows the UV-Vis absorbance of the date pit extracts and the MgO nanoparticles on a wavelength range 250-500 nm measured using a cary 5000 UV-Vis –NIR spectrophotometer. The absorbance peaks seen on the date pits extracts are characteristics of the contained phytochemicals. The appearance of the peak on the MgO nanoparticle is due to the phytochemiclas in the date pit extracts which favours the reduction of the Magnesium acetate resulting in the instant formation of MgO nanoparticles.



Figure s5: UV-Vis absorbance spectra for aqueous extracts of date pits and MgO nanoparticles

Figure s6 shows the PL spectra of the MgO nanoparticles annealed at 500℃ and 700℃. The morphology as well as the synthesis conditions of the MgO nanoparticles, resulted in two emission bands observed at 424 and 541 nm.



Figure s6: Photoluminescence spectra of the MgO annealed at 500° and 700°C

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| MgO (500°) | | | | | | |
| 2θ° | Miller index(hkl) | FWHM β° | d-spacing(Å) | nm | <˃nm | \*10-3 |
| 36.88 | (111) | 0.27 | 2.43 | 30.80 | 20.4 | 2.3 |
| 42.85 | (200) | 0.47 | 2.10 | 18.08 |
| 62.21 | (220) | 0.55 | 1.49 | 16.69 |
| 74.57 | (311) | 0.52 | 1.27 | 18.96 |
| 78.51 | (222) | 0.57 | 1.21 | 17.89 |

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| MgO(700°) | | | | | | |
| 2theta | Miller index | FWHM β° | d-spacing(Å) | nm | <˃nm | \*10-3 |
| 36.88 | (111) | 0.35 | 2.43 | 23.90 | 23.4 | 1.8 |
| 42.85 | (200) | 0.41 | 2.10 | 20.81 |  |  |
| 62.21 | (220) | 0.45 | 1.49 | 20.43 |  |  |
| 74.57 | (311) | 0.33 | 1.27 | 30.17 |  |  |
| 78.51 | (222) | 0.46 | 1.21 | 21.88 |  |  |

Table 1: Average particle size calculated from the XRD spectra according to the Debye–Scherrer formula. The different diffraction peaks gives different particle sizes

|  |  |  |  |
| --- | --- | --- | --- |
| Energy band gap (eV) | Bandgap of MgO | | |
| Un-annealed | Annealed at 500°C | Annealed at 700°C |
| 3.1 | 5.1 | 5.4 |
| Conduction band(eV) | 8.0 | 7.4 | 7.2 |
| Valence band (eV) | 11.1 | 12.5 | 12.5 |

Table 2: calculated MgO nanoparticles band gap and band edge potentials values

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Synthesis method | Morphology | Photocatalysis efficiency (%) | Bandgap(eV) | Ref |
| Green chemistry | spherical | 65 | 5.1 | Khan, et al.(2020) |
| Sol-gel | cubic | 38% | Didn’t record | Sierra-Fernandez et al. (2017) |
| Green chemistry | clusters of tiny, close-packed organization | 49.9 | 3.54 | Panchal et al.(2019) |
| Green chemistry | Spherical | 64 | 5.1 | Present work |

Table 3: Comparison of the physical and photocatalysis efficiency of the MgO nanoparticles with our work.

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