Title:	Tuning the hybridization and charge polarization in metal nanoparticles dispersed over Schiff base functionalized SBA-15 enhances CO2 capture and conversion to formic acid
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Abstract:	Different Schiff base functionalized SBA-15 materials were synthesized through condensation reactions between 3-aminopropyltriethoxysilane (APTES) and different aldehydes (glutaraldehyde and butyraldehyde) over a mesoporous silica, SBA-15 (APTES-GLU/SBA-15 and APTES-BUT/SBA-15). Both static and dynamic experiments have been used for testing the CO2 capture efficiency of these materials. The hybridization of the N atom in APTES has been tuned from sp3 to sp2 upon condensation facilitating optimum CO2 capture in the direct synthesis of APTES-GLU/SBA-15. The undesirable oxides of nitrogen have been removed during the synthesis process to improve the CO2 capture efficiency. These materials were employed as supports for Pd–Ag and Pd–Ni bimetallic systems for the selective conversion of the captured CO2 to formic acid (FA) in 0.5 M KHCO3 solution. The Pd–Ni catalyst system exhibited enhanced CO2 to FA conversion activity compared to other heterogeneous systems, which is ~4 times better than that of the Pd–Ag system in this study. The X-ray absorption studies over the catalyst material confirmed that the relatively electron-deficient Ni in Pd–Ni compared to Ag in Pd–Ag favoured higher charge polarization between the metals in the Pd–Ni system enhancing the CO2 to FA conversion. The experimental observations are well supported by the DFT calculations.
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