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The interaction of calcium, magnesium, lead, and cadmium cations with acidic/basic oxygen-containing groups on biochar surface: a DFT study.

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Biochar is a carbon-rich substance that has excellent adsorptive properties due to its porous structure, large surface area, and variable surface composition. By changing the functional groups present in biochar, the absorptivity of substances to the biochar can be modified. Calcium (Ca) and magnesium (Mg) are the major cations responsible for water hardness. Lead (Pb) and cadmium (Cd) are the major hazardous metal ions released into the water by industries. All these ions have various negative effects on living organisms. In this study, the interaction of the ions Ca and Mg with the biochar adsorbate was investigated with the use of Density Functional Theory (DFT) and semi-empirical calculations with the use of the GaussView 6.0 visualization program and Gaussian 09W quantum chemistry package. Seven biochar analogs were considered. Adsorbates with functional groups OH_2^+, $COOH_2^+$, OH, COOH, O^-, COO^- and the adsorbate with no functional groups were used in the calculations. Adsorption energies were calculated, which reflected the thermodynamic stability of the metal biochar complex. Two geometrical variations, in-plane and out of plane were considered. The average interatomic bond distance between Mg, and Ca with biochar adsorbate was found to be 3.865Å. Normalized binding energies were calculated for both geometrical variations. The most stable metal biochar complex was found to be analog number 07. Two analogs were unable to produce reasonable results. A significant deviation in normalized binding energy was seen in analog number 06. These results will pave a new path to get an insight into the adsorption of Ca, Mg, Pb, and Cd by biochar.

Keywords: Biochar, density functional theory, semi-empirical, adsorption energies, normalized binding energies