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'HWHUPLQDWLRQ RI S DUDEHQV LQ FRVPHWLF VDP SOHV XVLC
 KLJK SHUIRUPDQFH OLTXLG FKURPDWRJUDSK\ DQG XOWUDYL

\$VKRN .XPDU5DDPDLQGH,HSendX\$EXJDUandEHLQ QHWK²*)XUWRQ

¹Punjabi University, India

²)ORULGD ,QWHUQDWLRQDO 8QLYHUVLW\ 86\$

A simple, fast and sensitive analytical method using fabric phase sorptive extraction (FPSE) followed by high performance liquid chromatography ultraviolet detection (HPLC-UV) has been developed and validated for the extraction of parabens namely ethyl, methyl, propyl, butyl and benzyl paraben. Parabens are esters of p-hydroxybenzoic acid which are commonly used as preservatives in cosmetic products. Various factors affecting the performance of FPSE technique such as extraction time, eluting solvent, elution time and pH of the sample matrix were optimized. Determination was performed using reversed stationary phase C18 column with wavelength 254 nm. Separation was performed using mobile phase acetonitrile:water (63:37; v/v) at an isocratic flow rate of 1.0 mL/min. The calibration curves of the target analytes were prepared with good correlation coefficient values ($R^2 > 0.992$). The limit of detection (LOD) values range from 0.192-0.225 ng/mL and the developed method was applied successfully for the analysis of parabens in various cosmetic samples such as rose water, deodorant, serum and cream with extraction recoveries found in between 88% to 114%.

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Two-dimensional materials can be used in a variety of bioanalytical techniques. Interest in two-dimensional (2D) forms of Si and Ge has surged recently, with a focus on silicene and germanene, the Si- and Ge-based analogues of graphene as well as their derivatives. Siloxene and germoxene are 2D materials made of honeycomb Si and Ge backbone sheets that are decorated with H atoms and OH groups. This work uses first-principles calculations to probe the properties of their various conformations. It is shown that the most stable siloxene (and germoxene) polymorph is the so-called washboard structure, and not the chair geometry assumed in previous studies. The stability of the washboard conformation relates to the formation of a network of hydrogen bonds between its hydroxyl groups. It is also found with hybrid functional calculations that siloxene and germoxene are wide band-gap semiconductors with gap values of 3.20 eV and 2.64 eV, respectively. Finally, we show that H and OH vacancies introduce spin polarization in these 2D materials and have a tendency to pair up in stable di-vacancies.

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