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**'development and applications of the lfdf the non**

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periodic images of the eu 2 impurity 4 k points were included in each direction of the lattice'

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June 14th, 2019 - the g tensors and hfcs were obtained employing the hybrid functional b3lyp 61 63 the cp ppp basis set was applied for cu 64 while the tzvp basis set was used for sulfur 65 all other atoms were described employing the epr ii basis set 66 first order hfcs were calculated for 1 h and 14 n while spin orbit contributions were taken'

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June 4th, 2020 - graphene ? ? r æ f i? n is an allotrope of carbon in the form of a single layer of atoms in a two dimensional hexagonal lattice in which one atom forms each vertex it is the basic structural element of other allotropes including graphite charcoal carbon nanotubes and fullerenes it can also be considered as an indefinitely large

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**'orbits and orbitals chemguide**

**June 4th, 2020 - an orbital is just a bit of space where there is a 95 chance of finding that particular electron if an electron is in a particular orbital you know about its energy but there is no way of knowing how it is moving around within that orbital the big problem in all of this to my mind is the confusion in the words orbit and orbital'**

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**'turbomole modular program suite for ab initio quantum**

**June 4th, 2020 - from turbomole s beginnings code development was acpanied by basis set development an overview with typical applications for the different basis set families developed with turbomole is given in table i the turbomole or karlsruhe basis set family currently consists of four types the now outdated def basis sets 20 114 116 20 k'**

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