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Antiferromagnetic ordering in one-dimensional dangling-bond wires on a hydrogen-terminated C(001) surface

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We predict the existence of antiferromagnetic ordering in the one-dimensional dangling-bond wires fabricated on a hydrogen-terminated C(001) surface. Our spin-polarized density-functional theory calculations show that the antiferromagntic configuration, where the spins of adjacent dangling bonds point in opposite directions, is favored over the ferromagnetic one. Using the broken symmetry method, we estimate an exchange coupling constant of ~31 meV between adjacent spins. It is thus shown that unpaired electrons in sp^3-bonded diamond yield magnetic moments which interact antiferromagnetically with each other.