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The Donor/Acceptor Edge-Modification: An Effective Strategy to Modulate the Electronic and Magnetic Behaviors of Zigzag Silicon Carbon Nanoribbons

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It is known that the edge modification with electron donor/acceptor group can break the energy degeneracy between ferromagnetic (FM) and antiferromagnetic (AFM) states of the pristine zSiCNR, and the sole intriguing half-metallicity or metallicity corresponding to the ground state of FM/AFM can be achieved in the decorated 8-zSiCNR, as discussed in detail at the text. Besides, here we also provided electronic and magnetic properties of the parallel AFM (FM) state corresponding to the ground state of FM (AFM) for the studied systems with the unilateral/bilateral modification, where FM metal, AFM metal and AFM half-metal can also be observed, as shown in Tables S1 and S2, as well as Figures S1, S2, S3 and S4.

Table S1. The magnetic state, the electronic property and the band gap in minority channel of the parallel state corresponding to the ground state for the unilateral modified zSiCNRs.

System	Magnetic state	Electronic property	the gap in minority channel (eV)
H-zSiCNR-CN	FM	metal	-
CN-zSiCNR-H	FM	metal	-
H-zSiCNR-NO_2	AFM	half-metal	0.305
NO_2-zSiCNR-H	AFM	half-metal	0.283
H-zSiCNR-CH_3	AFM	half-metal	0.361
CH_3-zSiCNR-H	AFM	half-metal	0.449
H-zSiCNR-OH	AFM	half-metal	0.064
OH-zSiCNR-H	AFM	half-metal	0.364
H-zSiCNR-NH_2	FM	metal	-
NH_2-zSiCNR-H	AFM	half-metal	0.441

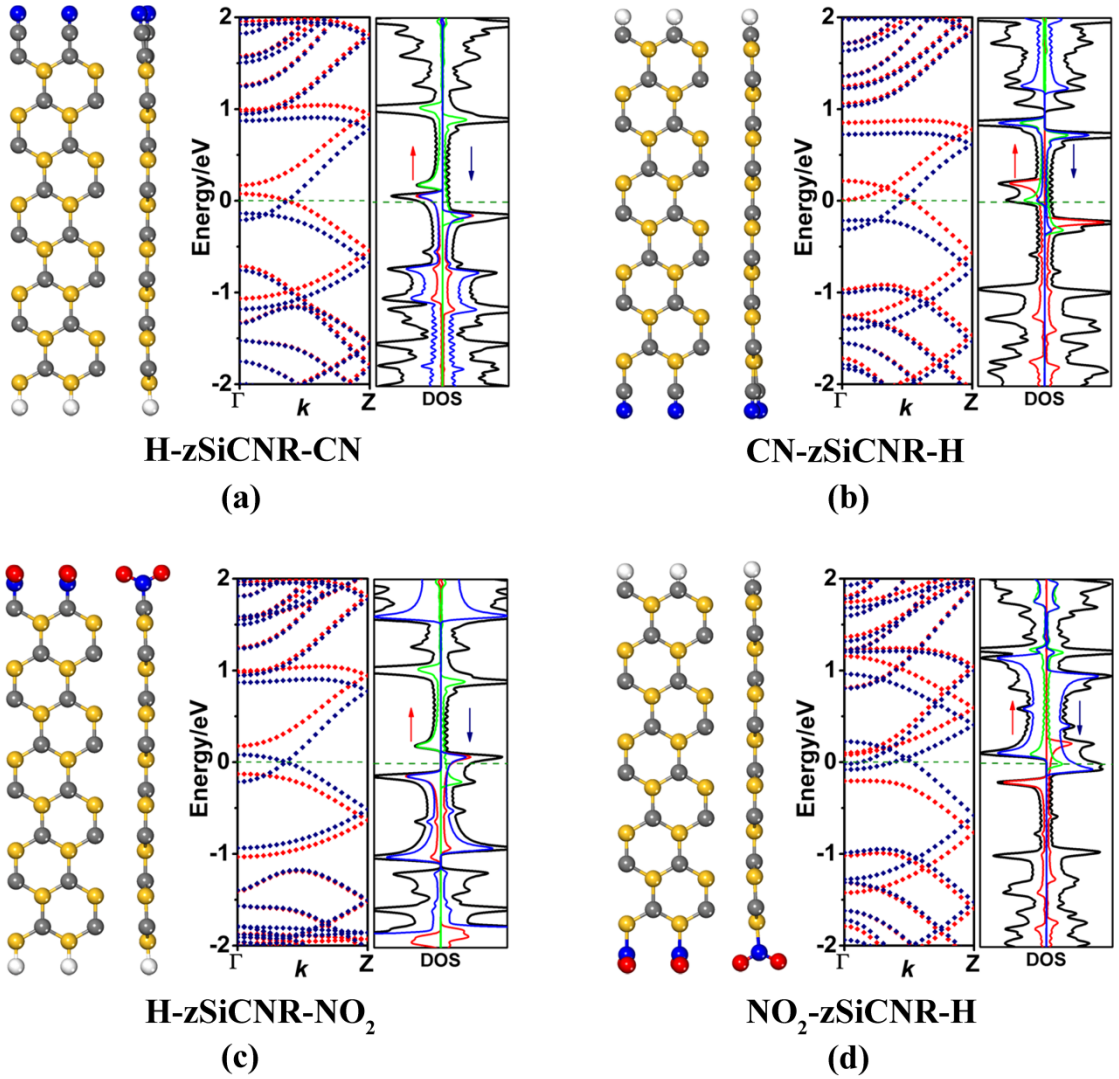

Figure S1. The geometries, electronic band structures, and according DOSs of the parallel state corresponding to the ground state for the unilateral modified zSiCNRs by using the electron acceptor group, namely, CN and NO_2. The detailed marks about DOSs are the same as in Fig. 2.

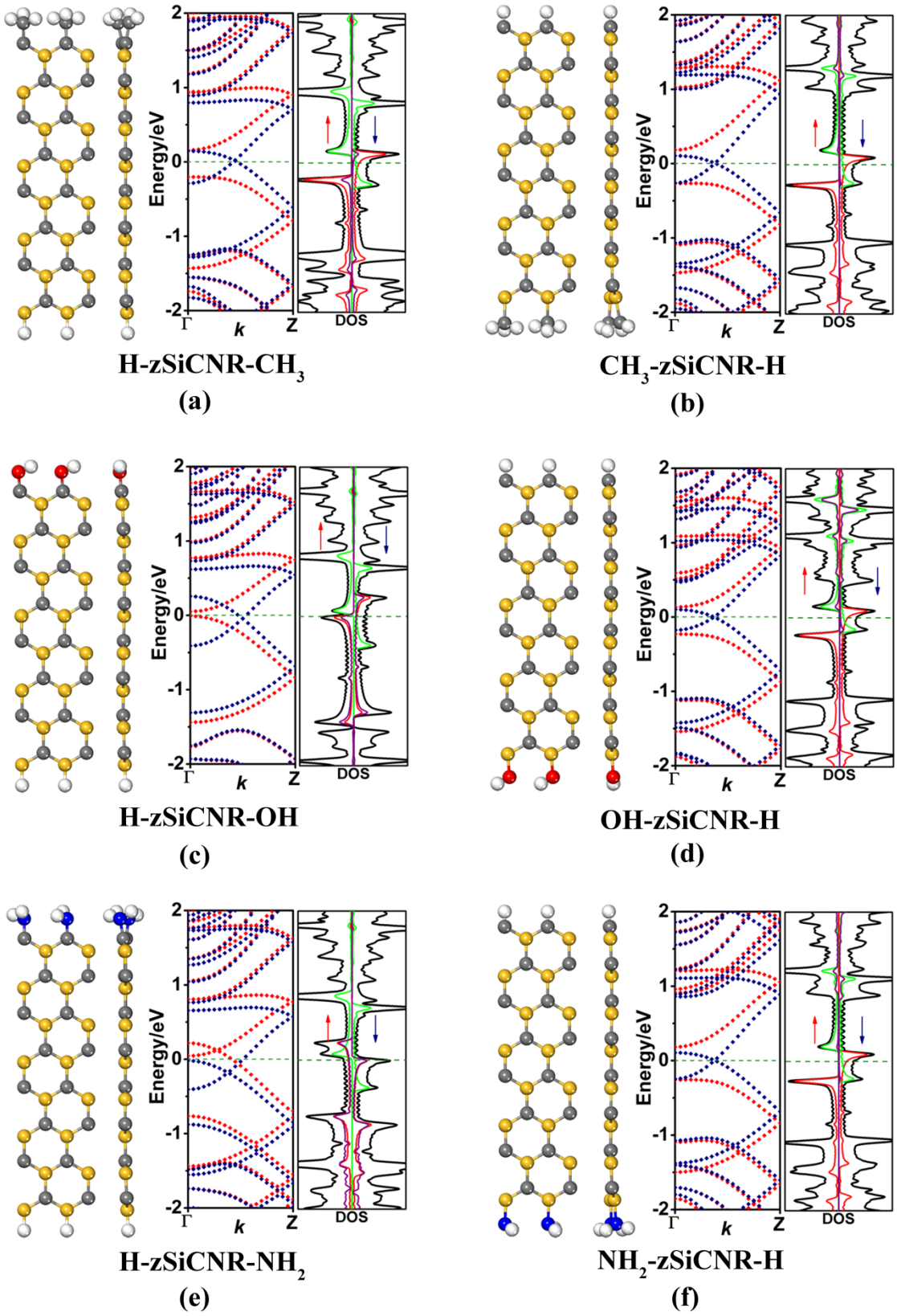

Figure S2. The geometries, electronic band structures, and according DOSs of the parallel state corresponding to the ground state for the unilateral modified zSiCNRs by using electron donor group namely, CH_3, OH and NH_2. The detailed marks about DOSs are the same as in Fig. 2.

Table S2. The magnetic state, the electronic property and the band gap in minority channel of the parallel state corresponding to the ground state for the bilateral modified zSiCNRs.

System	Magnetic state	Electronic property	the gap in minority channel (eV)
CH_3-zSiCNR-CN	AFM	half-metal	0.252
CN-zSiCNR-CH_3	AFM	metal	-
OH-zSiCNR-CN	AFM	half-metal	0.252
CN-zSiCNR-OH	AFM	metal	-
NH_2-zSiCNR-CN	FM	metal	-
CN-zSiCNR-NH_2	FM	metal	-
CH_3-zSiCNR-NO_2	AFM	half-metal	0.268
NO_2-zSiCNR-CH_3	AFM	half-metal	0.278
OH-zSiCNR-NO_2	AFM	half-metal	0.229
NO_2-zSiCNR-OH	AFM	metal	-
NH_2-zSiCNR-NO_2	AFM	half-metal	0.279
NO_2-zSiCNR-NH_2	FM	metal	-

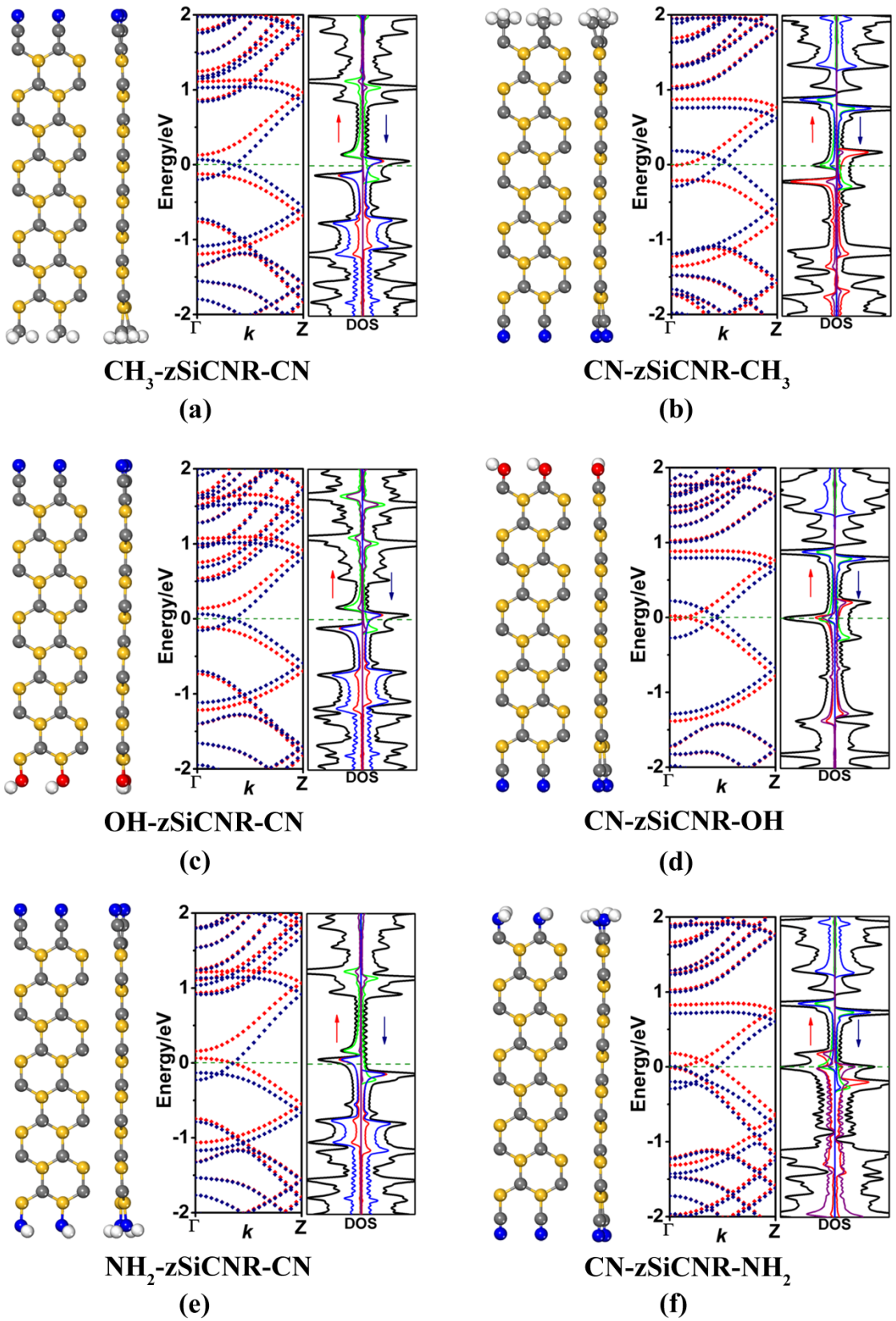

Figure S3. The geometries, electronic band structures, and according DOSs of the parallel state corresponding to the ground state for the bilateral modified zSiCNRs by using the electron accepter group CN and donor group CH_3, OH or NH_2. The detailed marks about DOSs are the same as in Fig. 2.

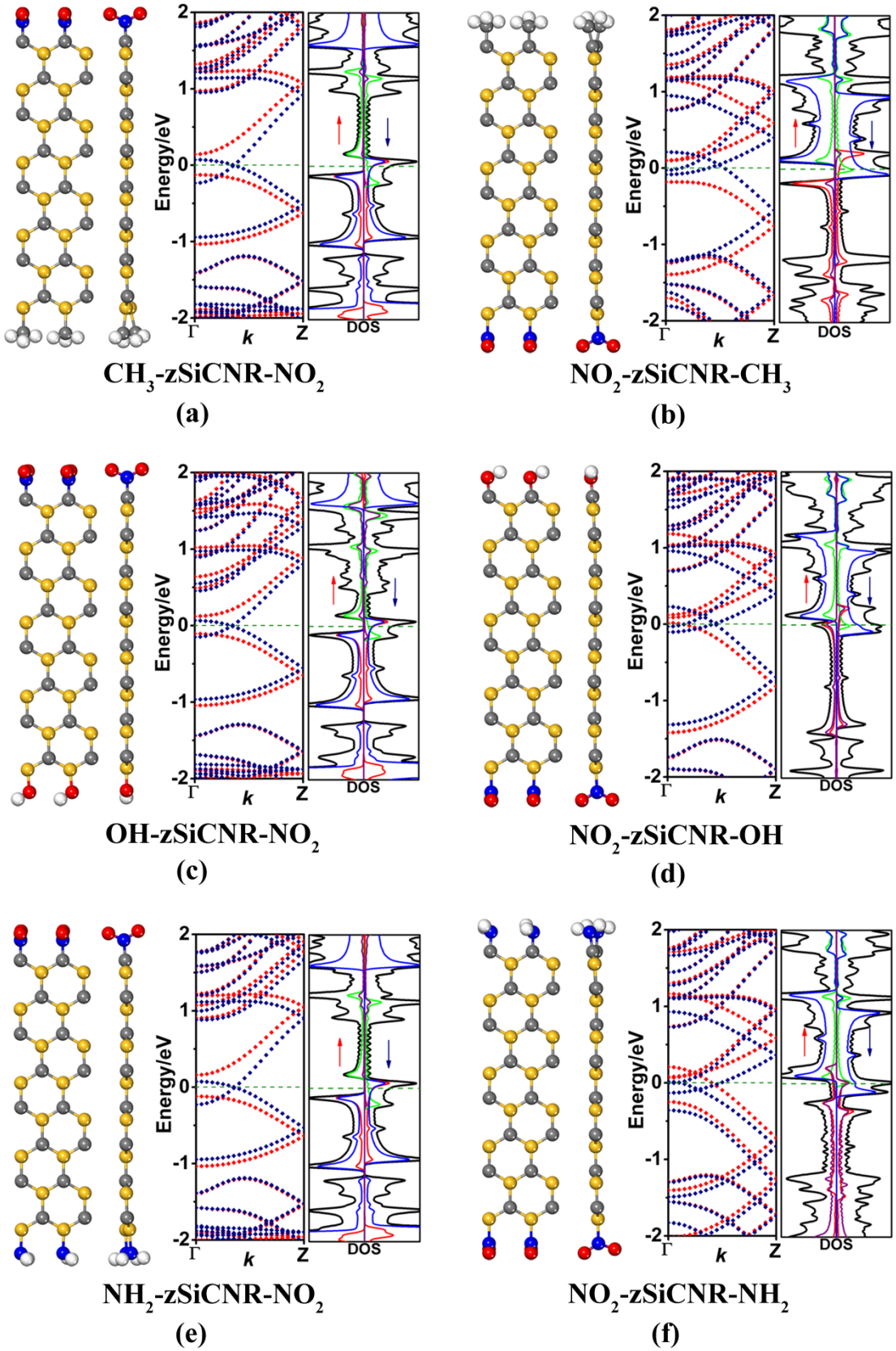

Figure S4. The geometries, electronic band structures, and according DOSs of the parallel state corresponding to the ground state for the bilateral modified zSiCNRs by using the electron accepter group NO_2 and donor group CH_3, OH or NH_2. The detailed marks about DOSs are the same as in Fig. 2.