

# Supporting Information

## From the Electron Density Gradient to the Quantitative Reactivity Indicators: Local Softness and the Fukui Function

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**Table S1.** Fukui functions for atoms and ions.

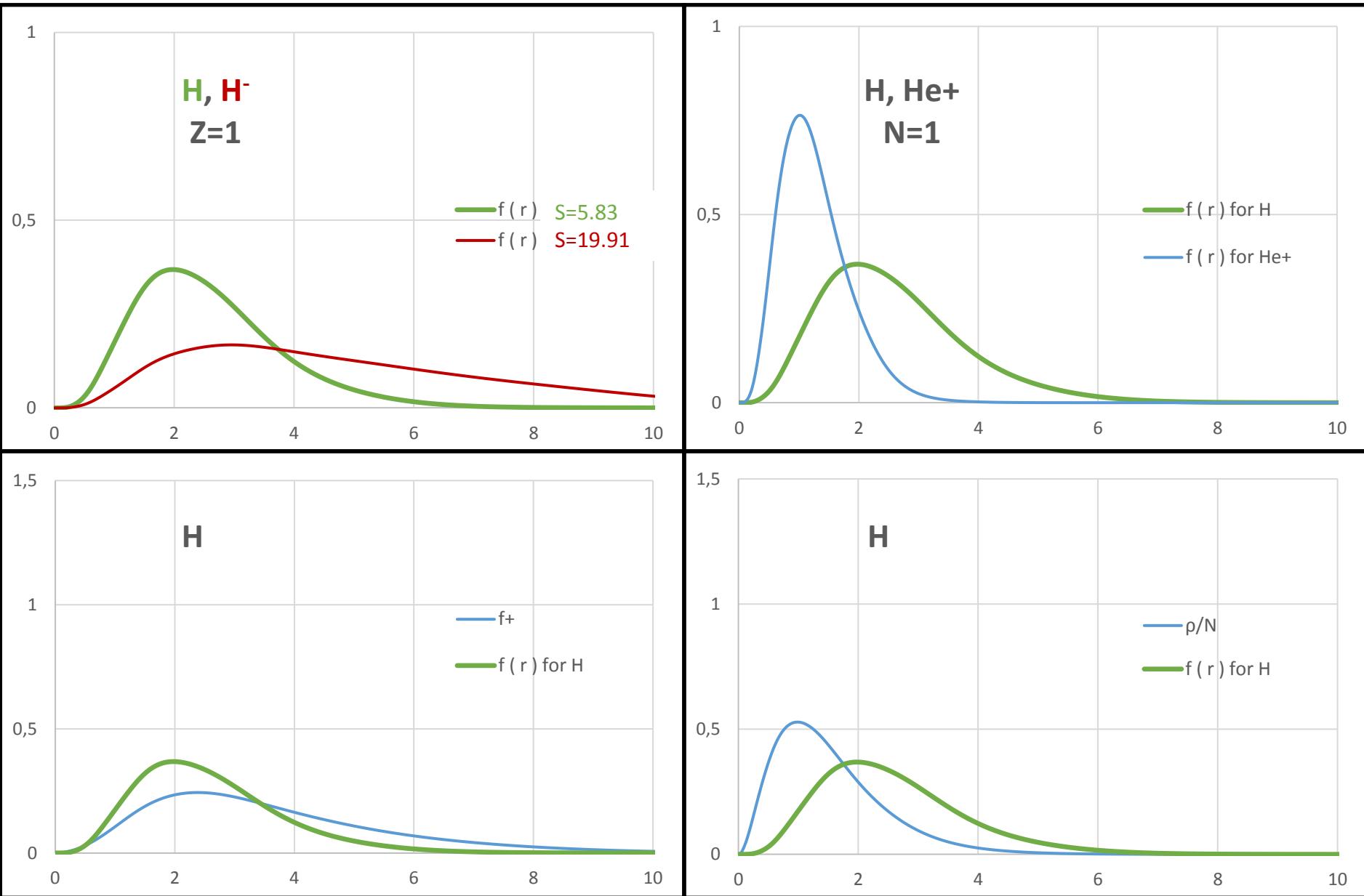
Graphical presentation of the radial distribution for the calculated Fukui function  $f(r)$  will open upon clicking on the atomic symbol.

H																He	
Li	Be																
Na	Mg																
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr

**Table S2** The presentation pattern for the atomic diagrams in Figures S1-S36 on pages S3-38  
All data are in atomic units [a.u].

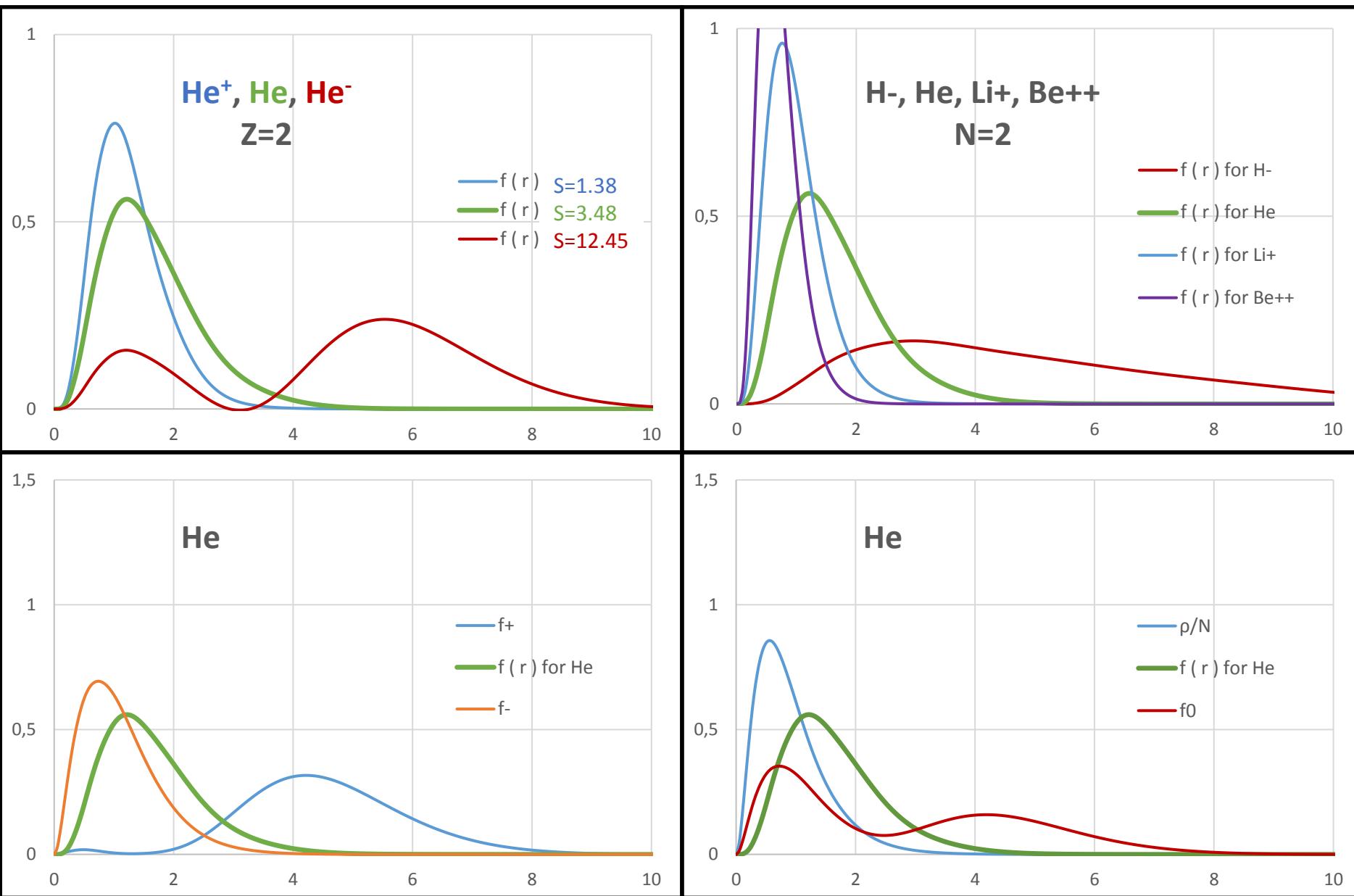
$f(r)$ and global softness for an atom and its selected ions	$f(r)$ for an atom and corresponding isoelectronic ions
$f(r)$ compared to $f^+(r)$ and $f^-(r)$	$f(r)$ compared to $f^o(r)$ and $\rho(r)/N$

Figure S1 Radial distribution for the calculated Fukui functions of H atom, its univalent ions and isoelectronic ions.



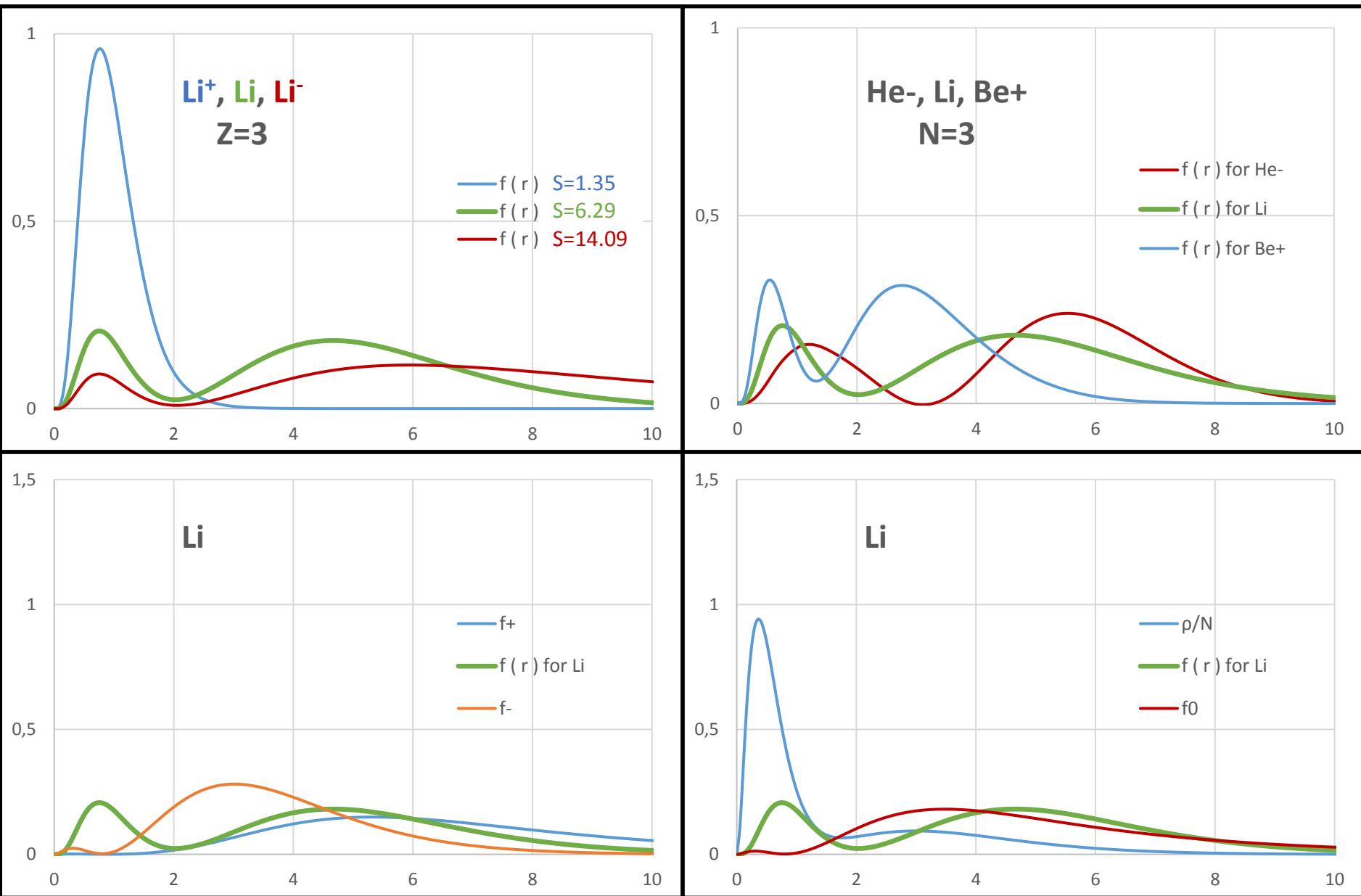
Li	Be		
C	N	O	F
Na	Mg		
Al	Si	P	Cl
Ca	Ge	As	Br
K	Ca	Sn	Kr
Sc	Ti	Zr	Rb
V	Cr	Mn	Te
Cr	Mn	Fe	Se
Mo	Ta	Co	Ni
Ta	W	Os	Pt
Re	U	Ru	Rh
W	Os	Ir	Pd
U	Th	Pt	Ag
He			

Figure S2 Radial distribution for the calculated Fukui functions of He atom, its univalent ions and isoelectronic ions.



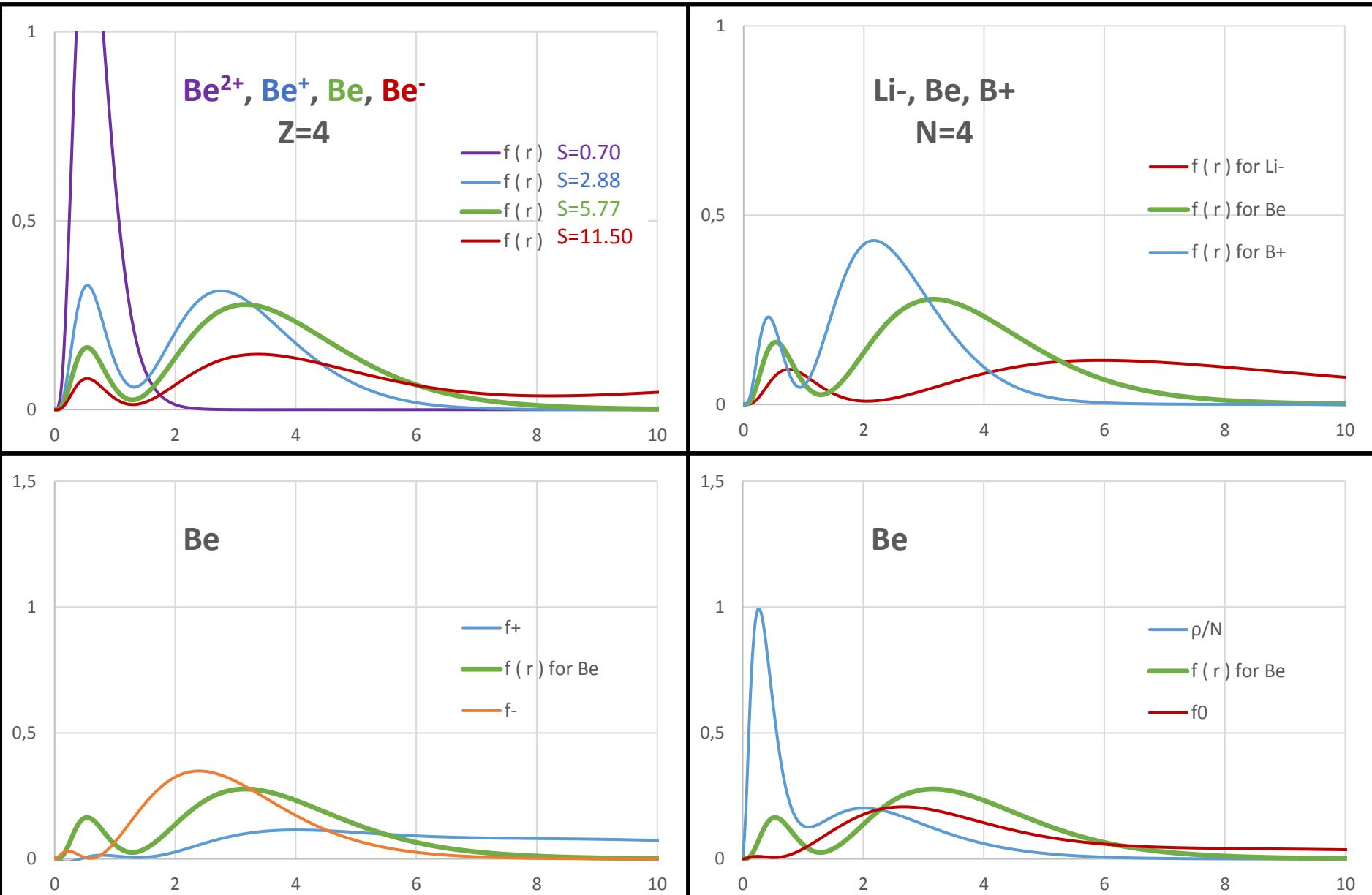
ELEMENTS	
H	He
Li	Be
B	C
C	N
O	F
N	Ne
P	Ar
S	Cl
Cl	Ar
Al	Si
Si	P
P	S
S	Cl
Cl	Ar
K	Ca
Ca	Sc
Sc	Ti
Ti	V
V	Cr
Cr	Mn
Mn	Fe
Fe	Co
Co	Ni
Ni	Cu
Cu	Zn
Zn	Ga
Ga	Ge
Ge	As
As	Se
Se	Br
Br	K

Figure S3 Radial distribution for the calculated Fukui functions of Li atom, its univalent ions and isoelectronic ions.



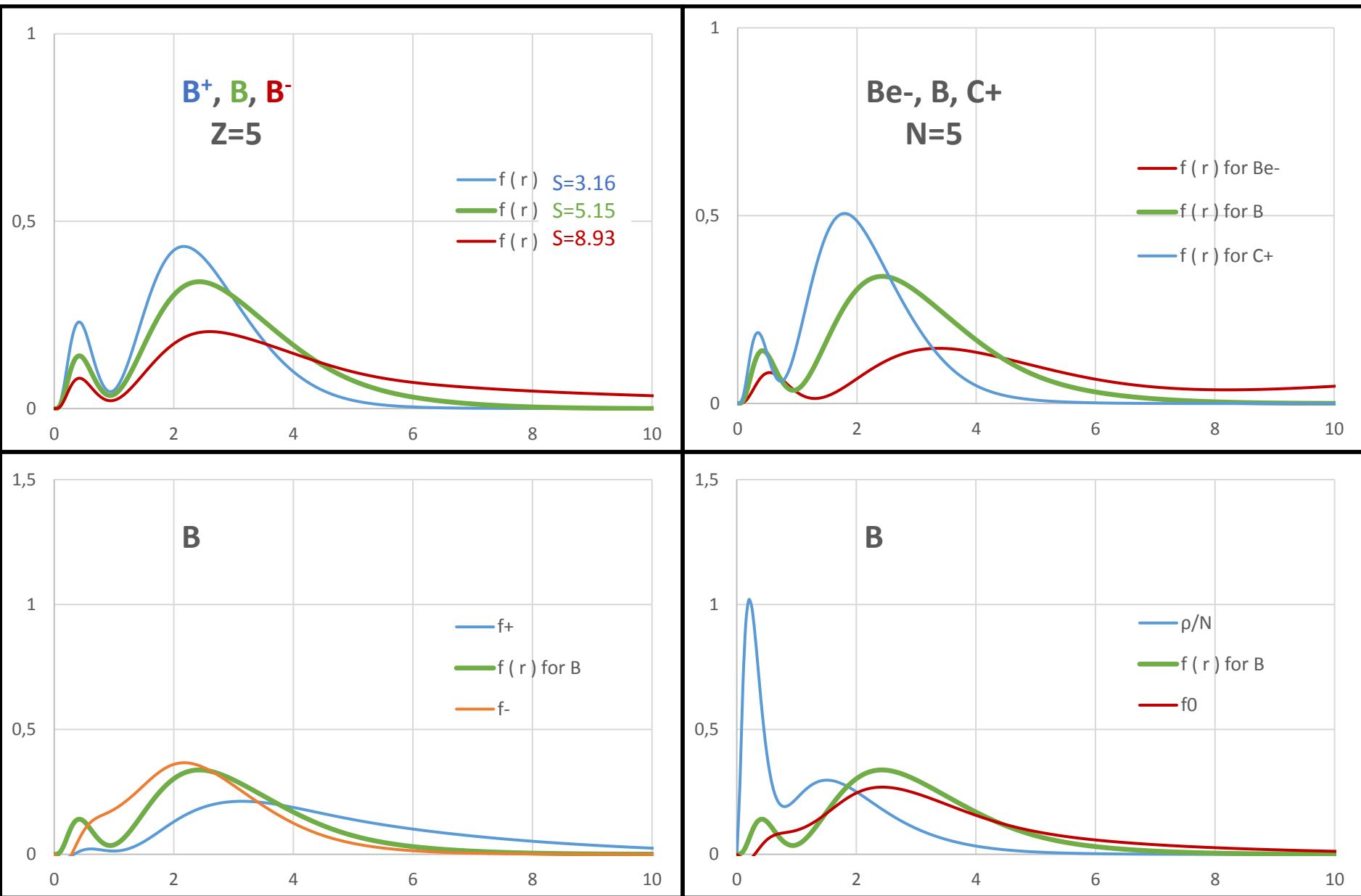
ELEMENTS	
$\text{H}$	$\text{He}$
$\text{Li}$	$\text{Be}$
$\text{B}$	$\text{C}$
$\text{N}$	$\text{O}$
$\text{F}$	$\text{Ne}$
$\text{Na}$	$\text{Mg}$
$\text{Al}$	$\text{Si}$
$\text{P}$	$\text{S}$
$\text{Cl}$	$\text{Ar}$
$\text{K}$	$\text{Ca}$
$\text{Sc}$	$\text{Ti}$
$\text{V}$	$\text{Cr}$
$\text{Mn}$	$\text{Fe}$
$\text{Co}$	$\text{Ni}$
$\text{Cu}$	$\text{Zn}$
$\text{Ga}$	$\text{As}$
$\text{Ge}$	$\text{Se}$
$\text{Br}$	$\text{Kr}$
$\text{Rb}$	$\text{Cs}$

Figure S4 Radial distribution for the calculated Fukui function of Be atom, its ions and isoelectronic ions.



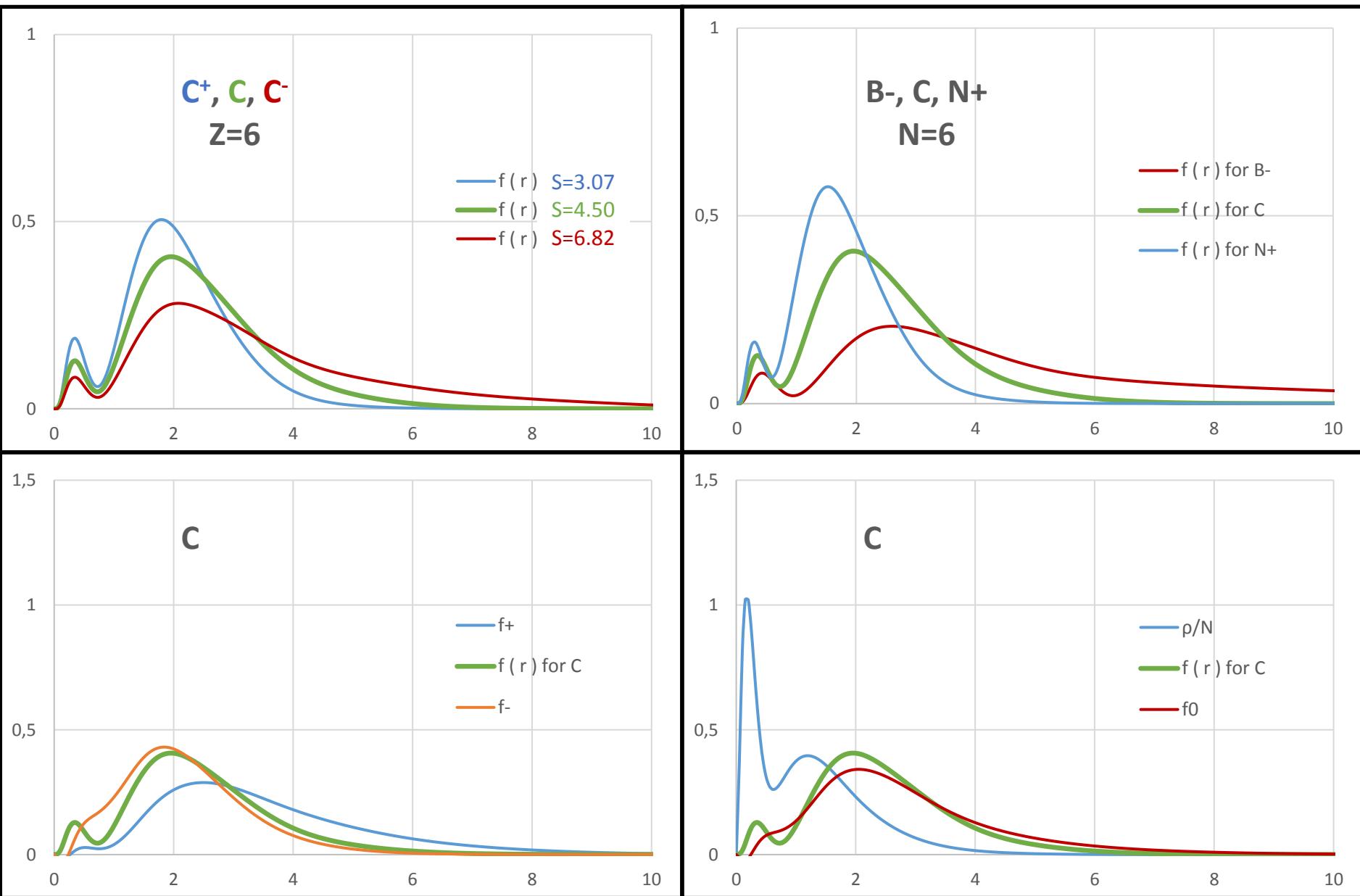
ELEMENTS	<table border="1"> <tr><td>H</td><td>He</td></tr> <tr><td>Li</td><td>Be</td></tr> <tr><td>B</td><td>C</td><td>N</td><td>O</td><td>F</td></tr> <tr><td>D</td><td>Ne</td></tr> <tr><td>K</td><td>Ca</td><td>Si</td><td>P</td><td>S</td><td>Cl</td></tr> <tr><td>Na</td><td>Mg</td><td>Al</td><td>Si</td><td>Ge</td><td>As</td><td>Br</td><td>K</td></tr> <tr><td>Sc</td><td>Ti</td><td>V</td><td>Cr</td><td>Mn</td><td>Co</td><td>Ni</td><td>Cu</td><td>Zn</td></tr> <tr><td>Ca</td><td>Sc</td><td>Al</td><td>Si</td><td>Ge</td><td>As</td><td>Br</td><td>K</td></tr> </table>	H	He	Li	Be	B	C	N	O	F	D	Ne	K	Ca	Si	P	S	Cl	Na	Mg	Al	Si	Ge	As	Br	K	Sc	Ti	V	Cr	Mn	Co	Ni	Cu	Zn	Ca	Sc	Al	Si	Ge	As	Br	K
H	He																																										
Li	Be																																										
B	C	N	O	F																																							
D	Ne																																										
K	Ca	Si	P	S	Cl																																						
Na	Mg	Al	Si	Ge	As	Br	K																																				
Sc	Ti	V	Cr	Mn	Co	Ni	Cu	Zn																																			
Ca	Sc	Al	Si	Ge	As	Br	K																																				

Figure S5 Radial distribution for the calculated Fukui functions of B atom, its univalent ions and isoelectronic ions.



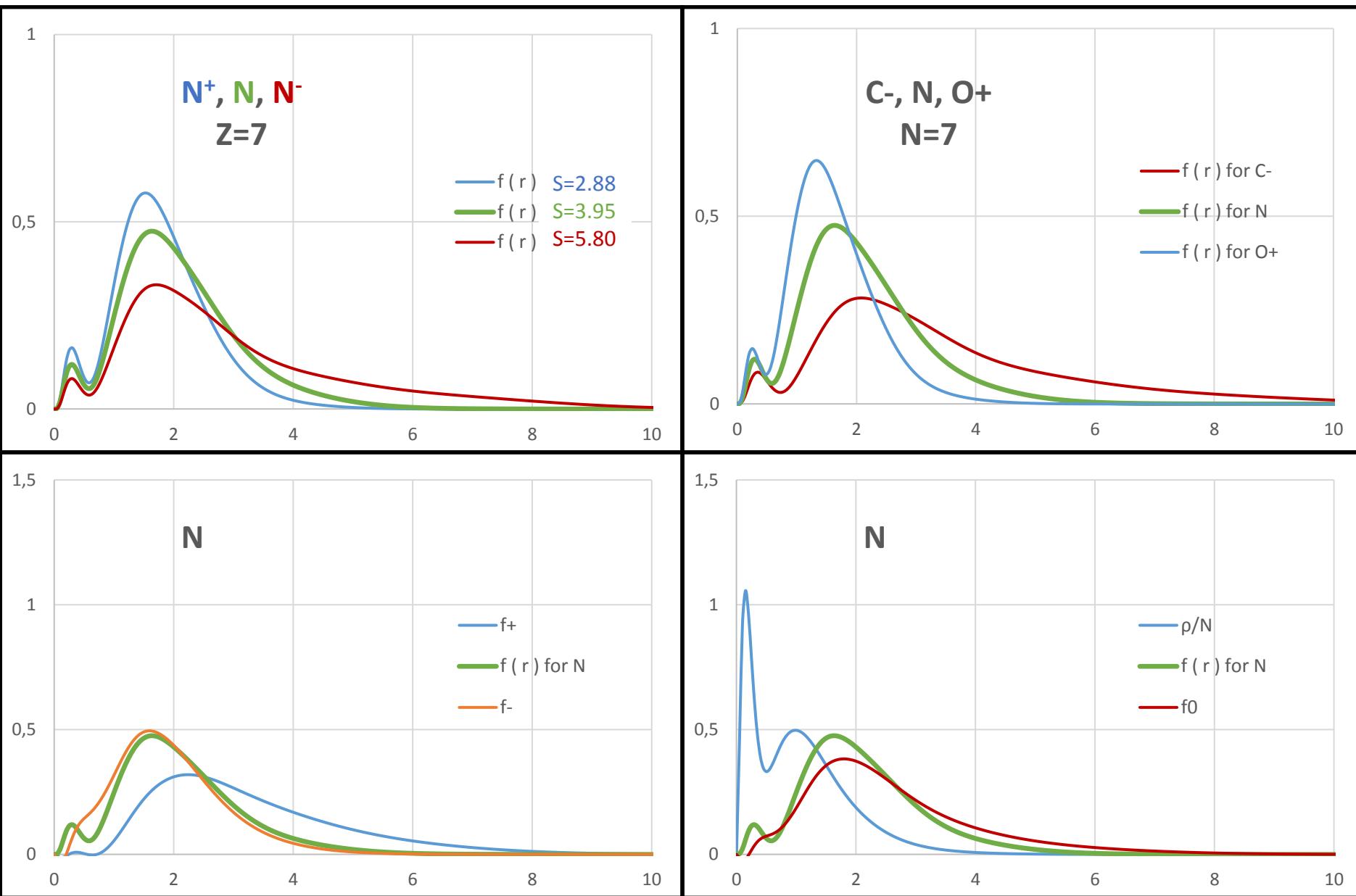
Li	Be	
Li	Be	
Be		
Ca		
K	Mg	

Figure S6 Radial distribution for the calculated Fukui functions of C atom, its univalent ions and isoelectronic ions.



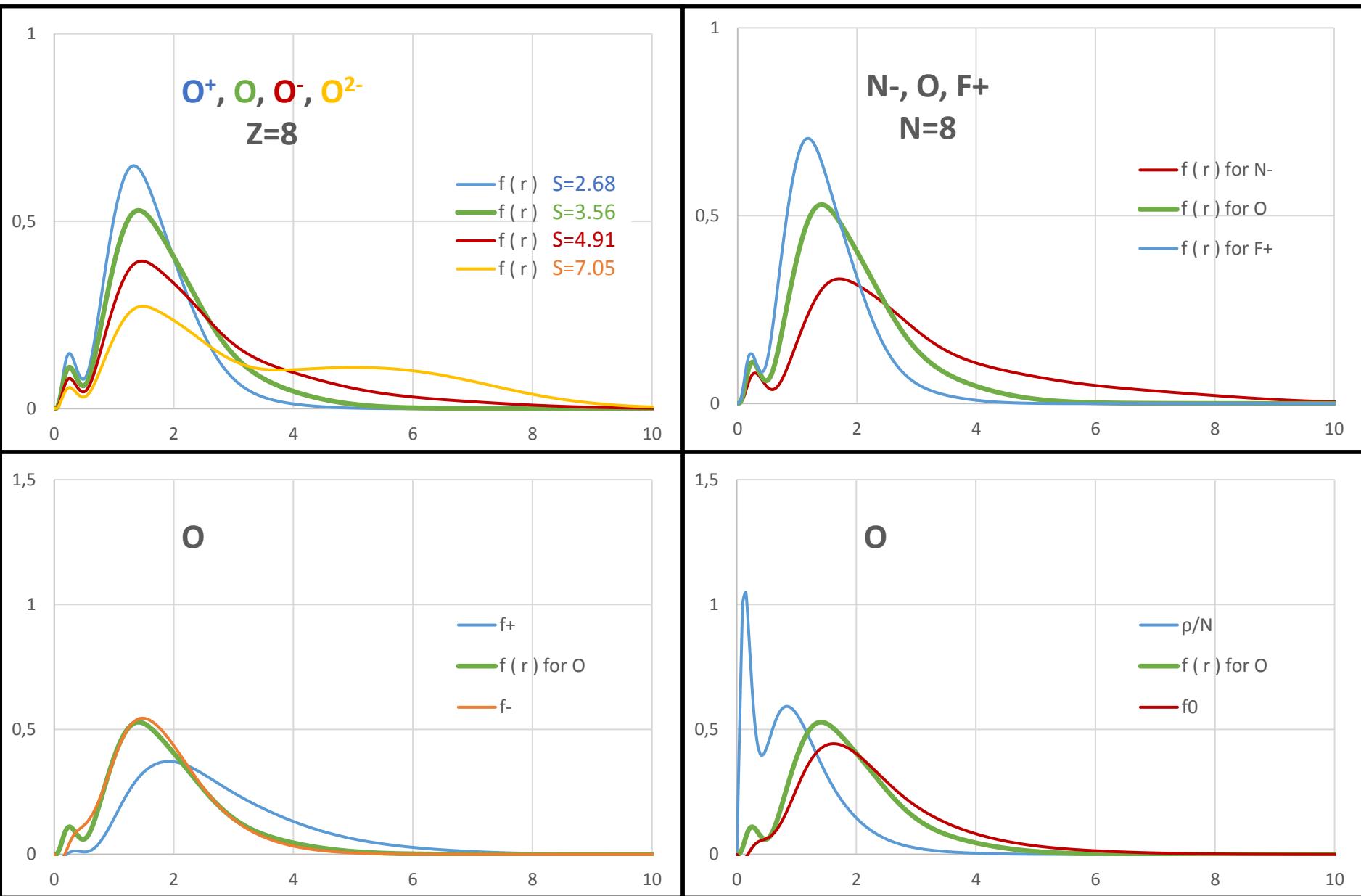
ELEMENTS	
H	He
Li	Be
B	C
N	O
F	Ne
Na	Mg
K	Ca
Sc	Ti
V	Cr
Mn	Fe
Co	Ni
Cu	Zn
Ga	Ge
As	P
Sb	Se
Br	Cl
I	Te

Figure S7 Radial distribution for the calculated Fukui functions of N atom, its univalent ions and isoelectronic ions.



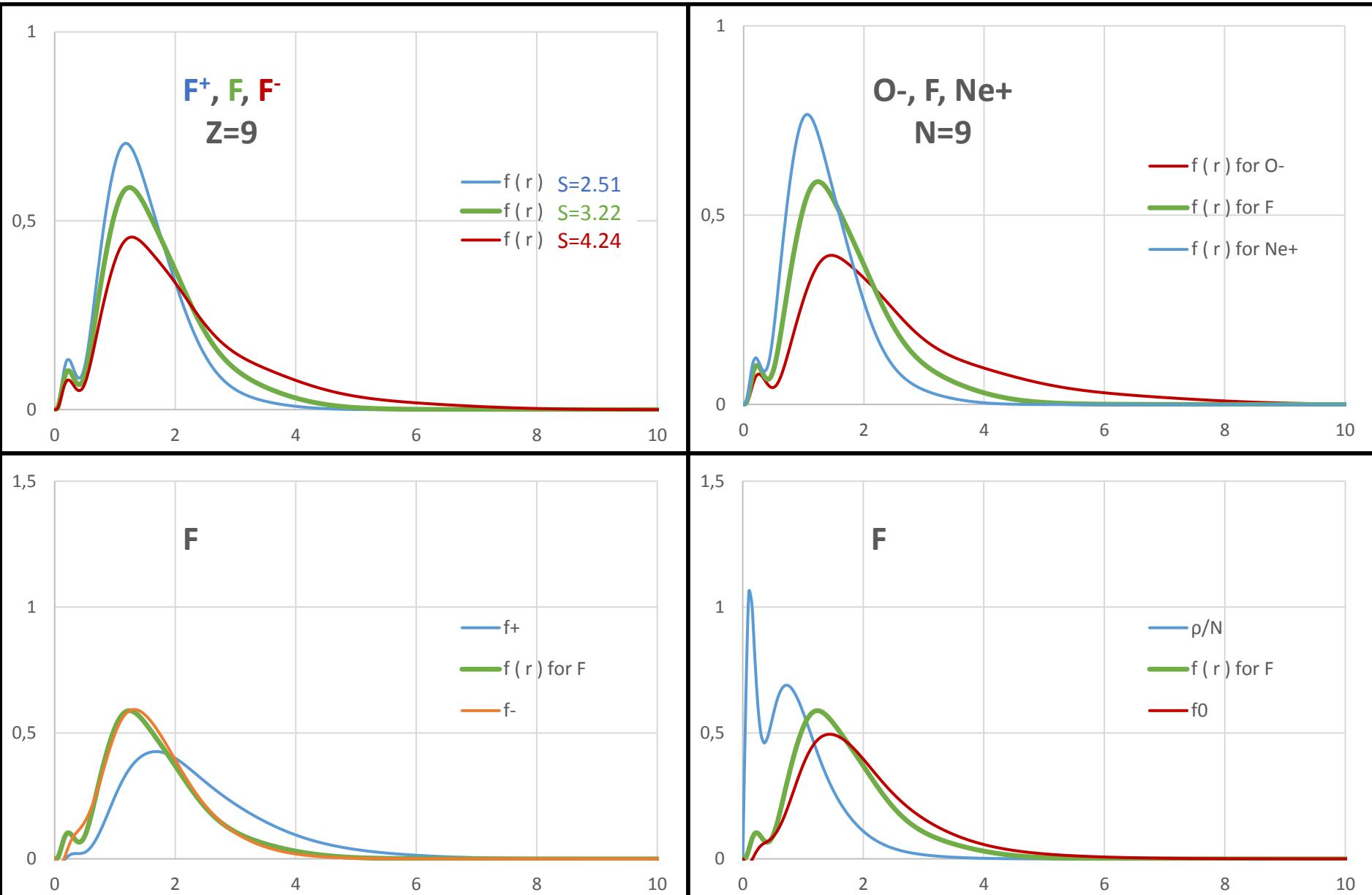
Li	Be	
B	C	N
Na	Si	O
K	Ca	F
Al	Si	P
Mg	Ca	S
Sc	Al	Cl
Ti	Si	Br
V	Al	K
Cr	Ca	
Mn	Ca	
Co	Si	
Ni	Al	
Cu	Cl	
Zn	Br	
Ga	K	
In		
Tl		

Figure S8 Radial distribution for the calculated Fukui function of O atom, its ions and isoelectronic ions.



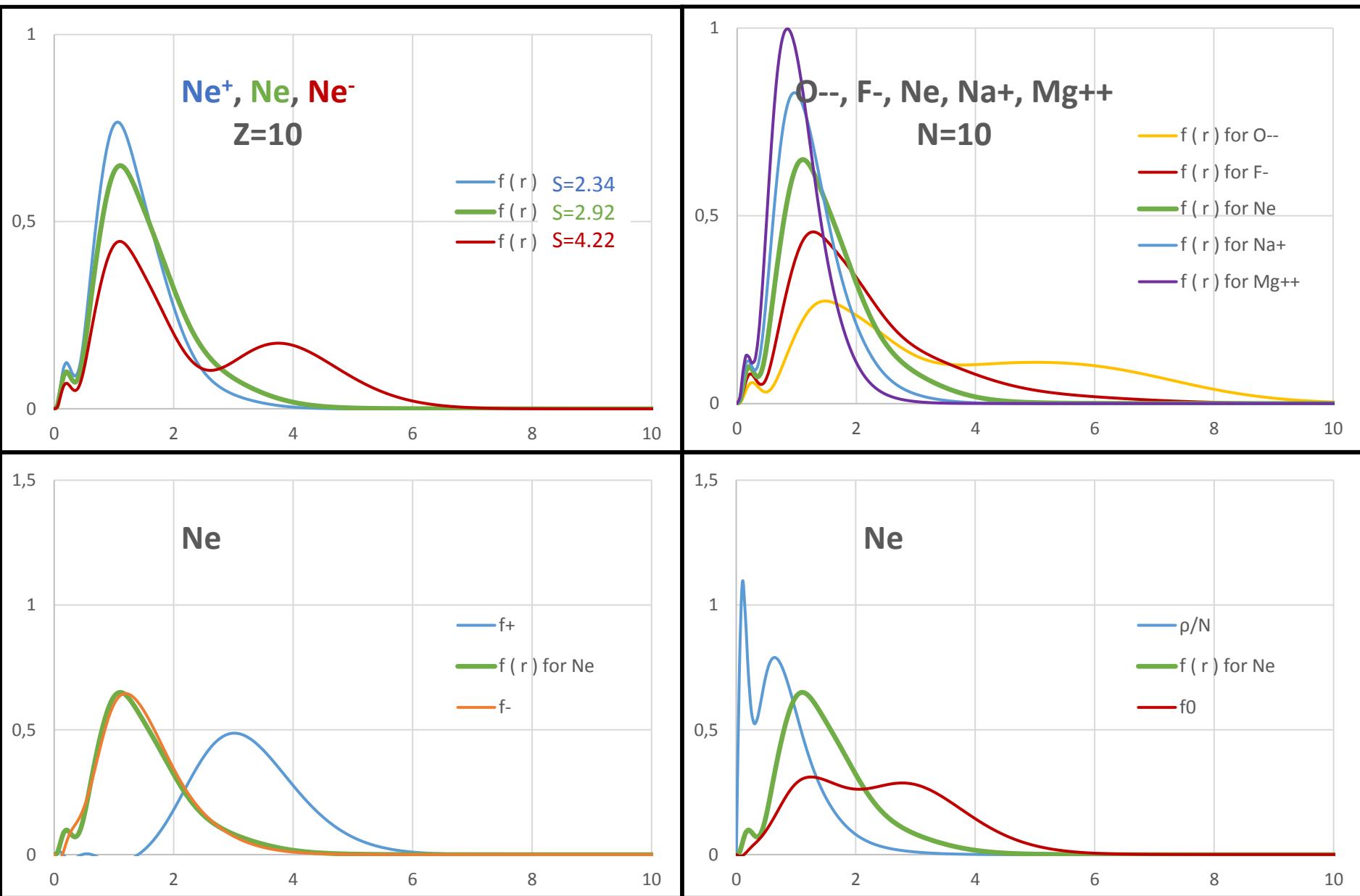
ELEMENTS	
H	He
B	C
N	O
F	Ne
Li	Be
Na	Mg
Al	Si
P	S
Cl	Ar
K	Ca
Sc	Ti
V	Cr
Cr	Mn
Fe	Co
Ni	Cu
Zn	Ge
Ga	As
In	Se
Tl	Br
Pb	I

Figure S9 Radial distribution for the calculated Fukui functions of F atom, its univalent ions and isoelectronic ions.



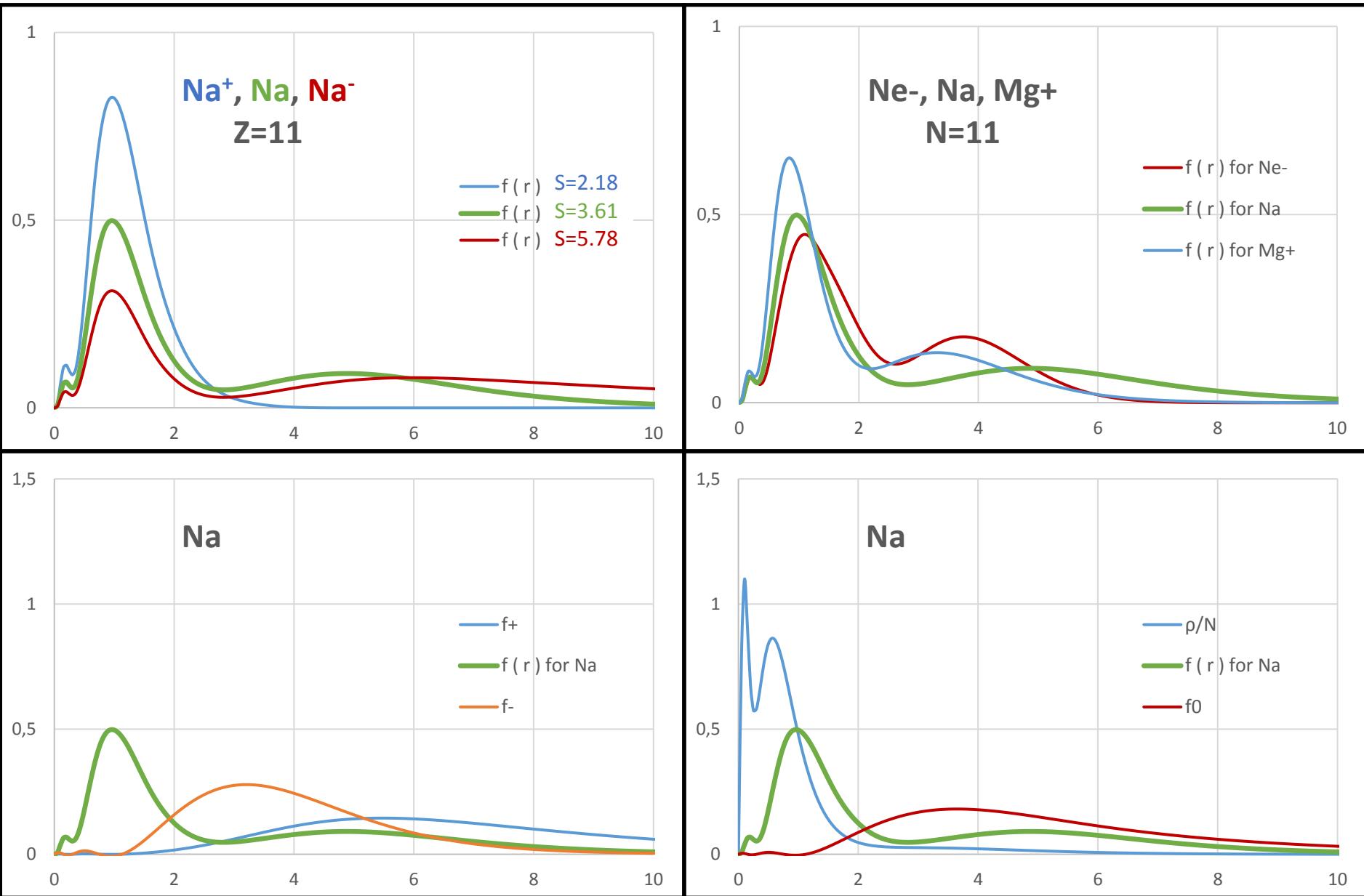
ELEMENTS	
H	He
Li	Be
B	C
C	N
N	O
O	F
F	Ne
Na	Mg
K	Ca
Al	Si
Si	P
P	S
S	Cl
Cl	Ar
Ar	Br
Br	Kr

Figure S10 Radial distribution for the calculated Fukui functions of Ne atom, its univalent ions and isoelectronic ions.



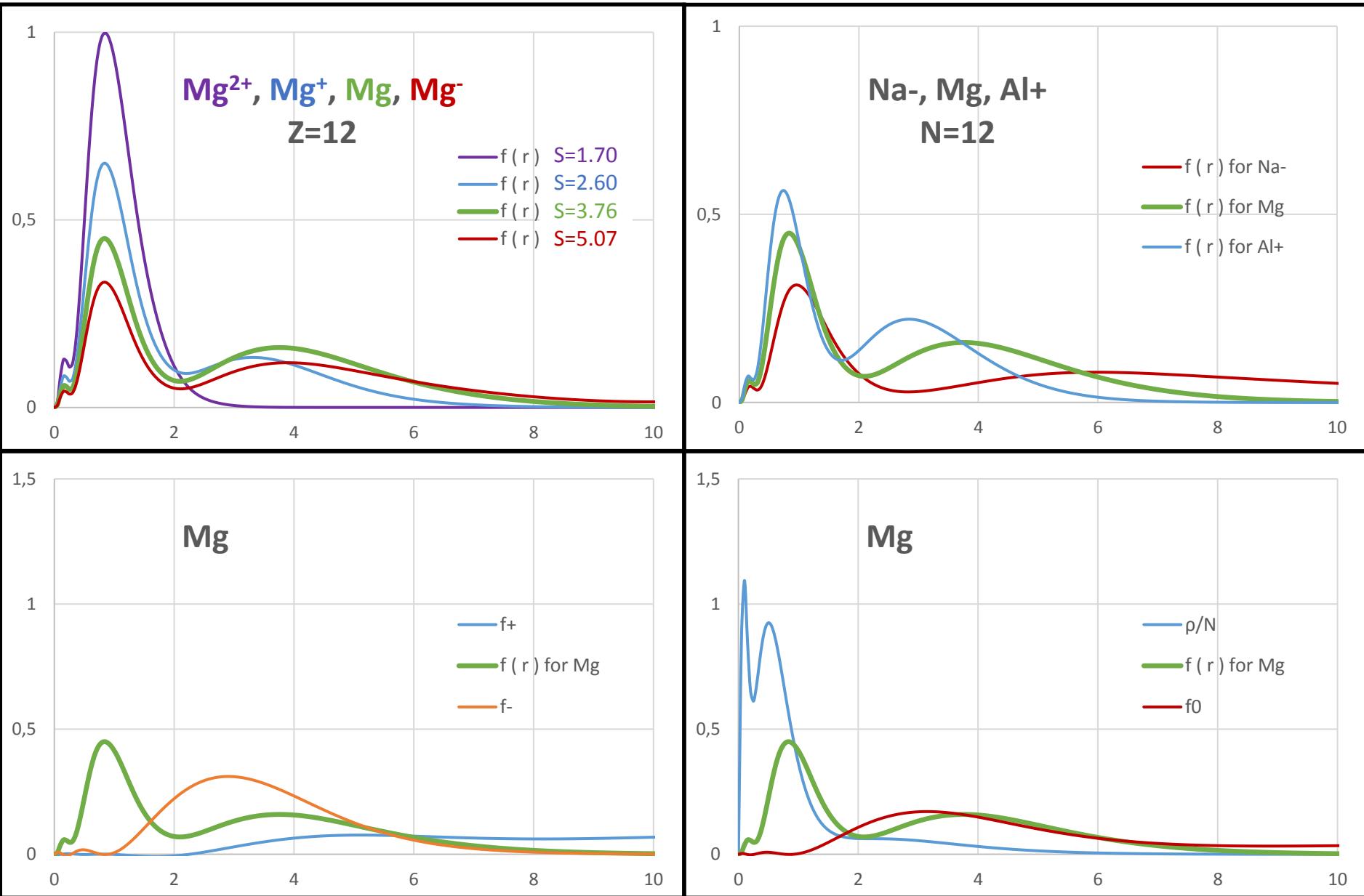
ELEMENTS	
H	He
Li	Be
B	C
N	O
F	Ne
Na	Mg
K	Ca
Sc	Ti
V	Cr
Cr	Mn
Ta	Co
Co	Ni
Cu	Zn
Ga	Ge
As	P
S	Cl
Br	Ar
Kr	Rb

Figure S11 Radial distribution for the calculated Fukui functions of Na atom, its univalent ions and isoelectronic ions.



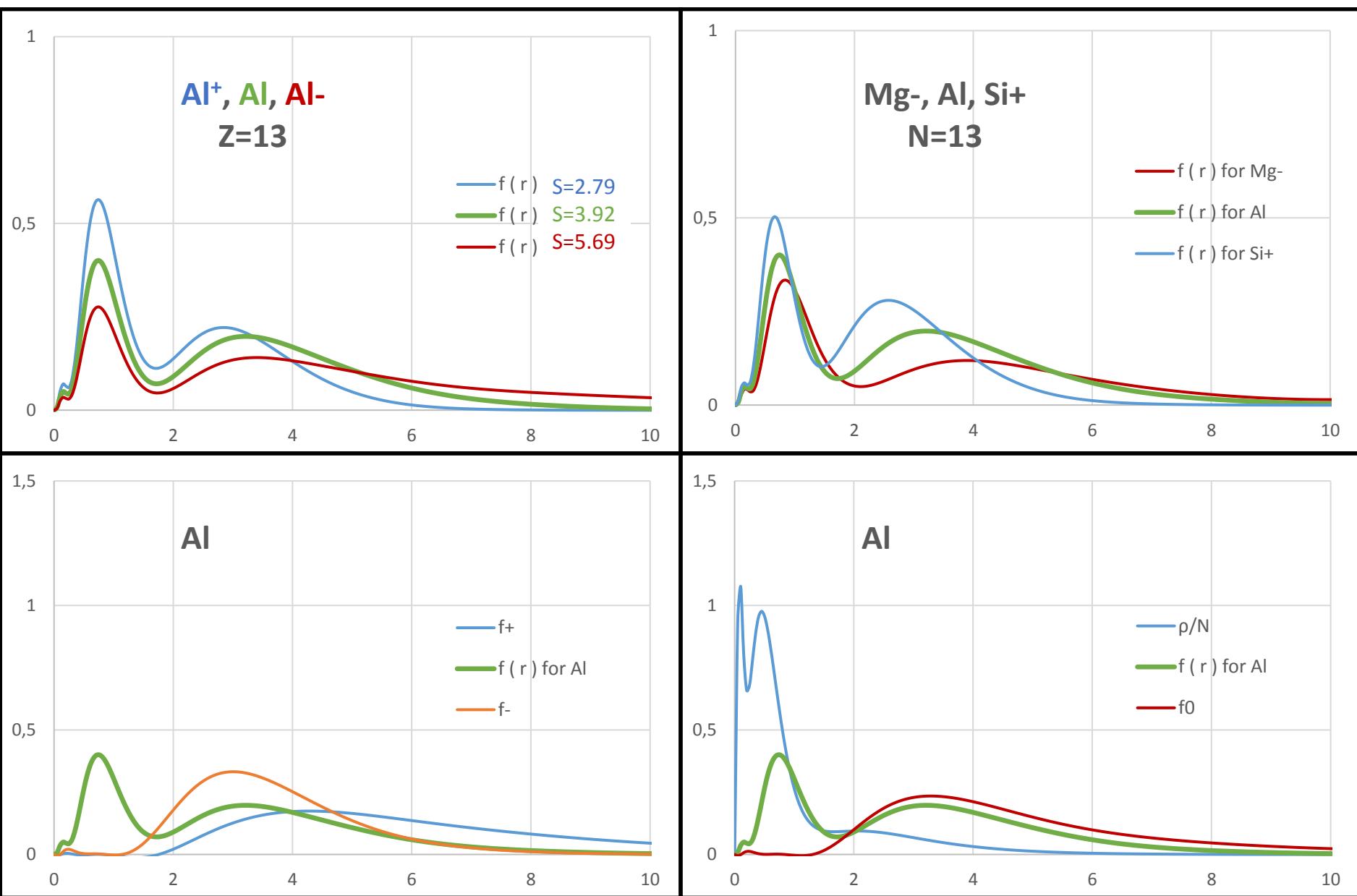
Li	Be	ELEMENTS			B	C	N	O	F
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni

Figure S12 Radial distribution for the calculated Fukui functions of Mg atom, its ions and isoelectronic ions.



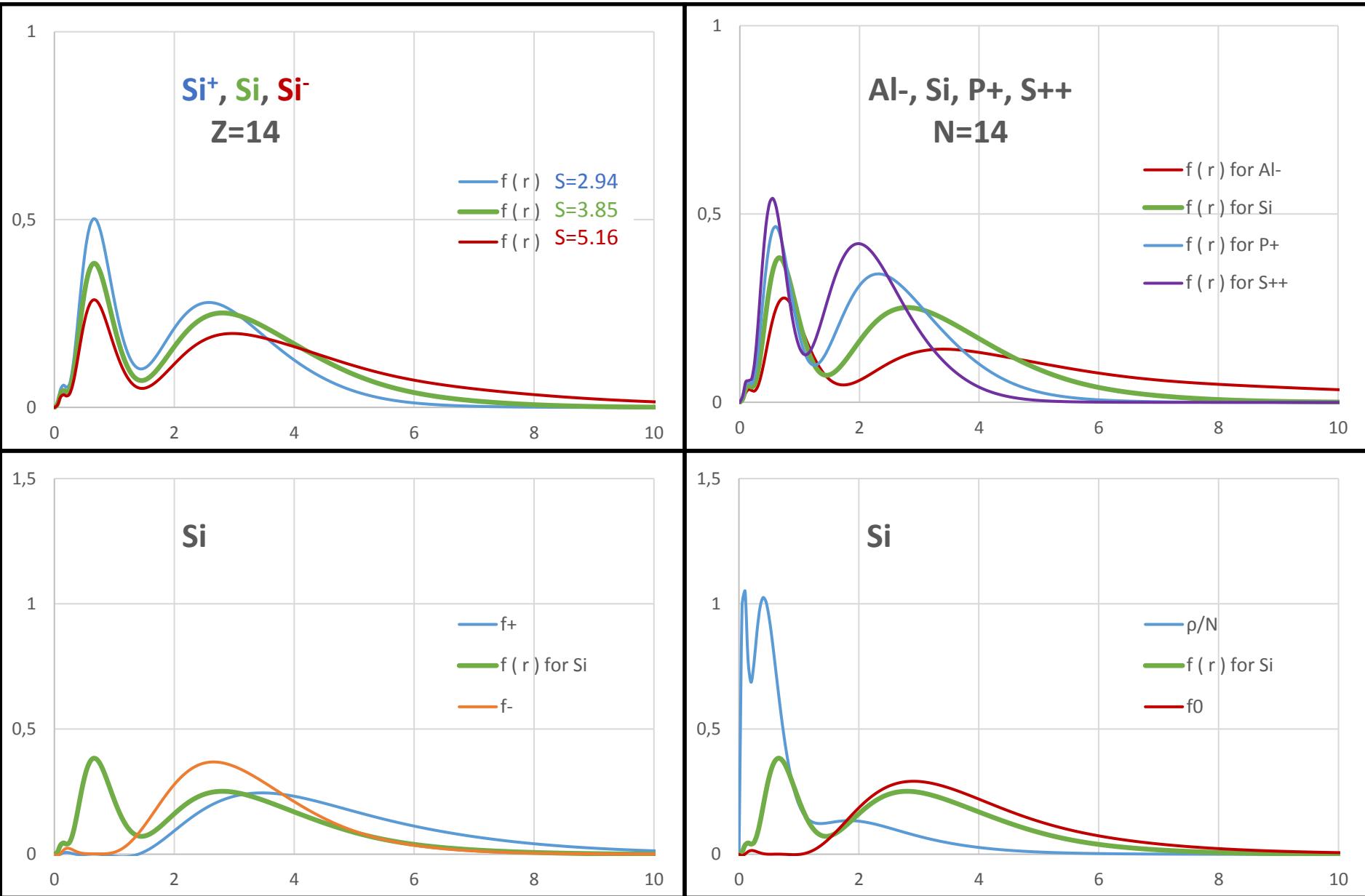
ELEMENTS	
H	He
Li	Be
B	C
C	N
N	O
O	F
F	Ne
Na	Mg
Mg	Al
Al	Si
Si	P
P	S
S	Cl
Cl	Ar
K	Ca
Ca	Sc
Sc	Ti
Ti	V
V	Cr
Cr	Mn
Mn	Fe
Fe	Co
Co	Ni
Ni	Cu
Cu	Zn
Zn	Ga
Ga	In
In	Tl
Tl	Br
Br	Kr

**Figure S13 Radial distribution for the calculated Fukui functions of Al atom, its univalent ions and isoelectronic ions.**



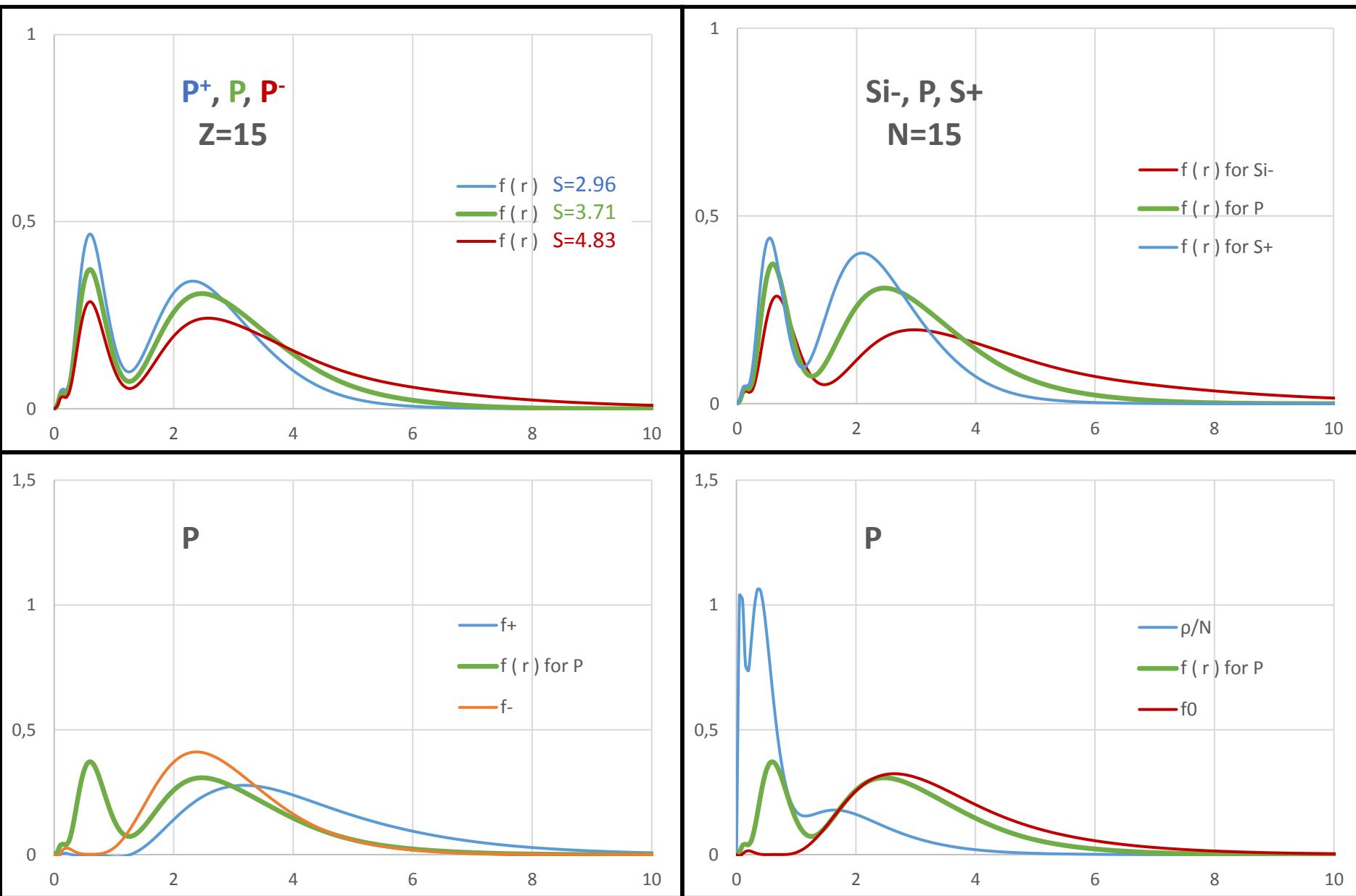
ELEMENTS	
H	He
Li	Be
B	C
N	O
F	Ne
Na	Mg
K	Ca
Sc	Ti
V	Cr
Cr	Mn
Ta	Co
Co	Ni
Cu	Zn
Ge	P
As	S
Se	Cl
Br	Kr

Figure S14 Radial distribution for the calculated Fukui functions of Si atom, its univalent ions and isoelectronic ions.



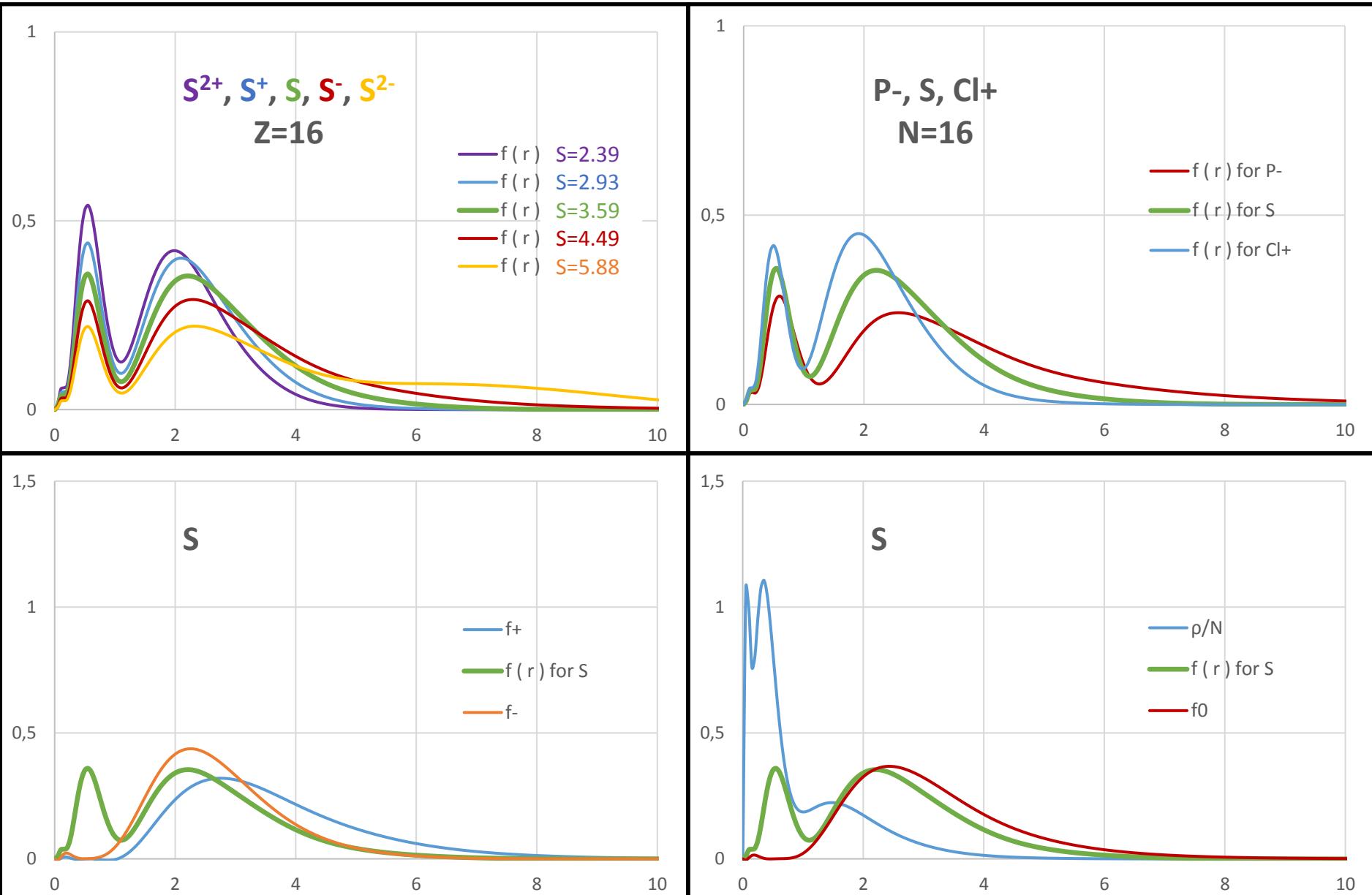
Li	Be	
Li	Be	
Na	Mg	
K	Ca	
Sc	Ti	
V	Cr	
Cr	Mn	
Co	Ni	
Cu	Zn	
Ag	Pd	
Ca	Ge	
Br	As	
Kr	Cl	
Ca	Br	
Br	K	

Figure S15 Radial distribution for the calculated Fukui functions of P atom, its univalent ions and isoelectronic ions.



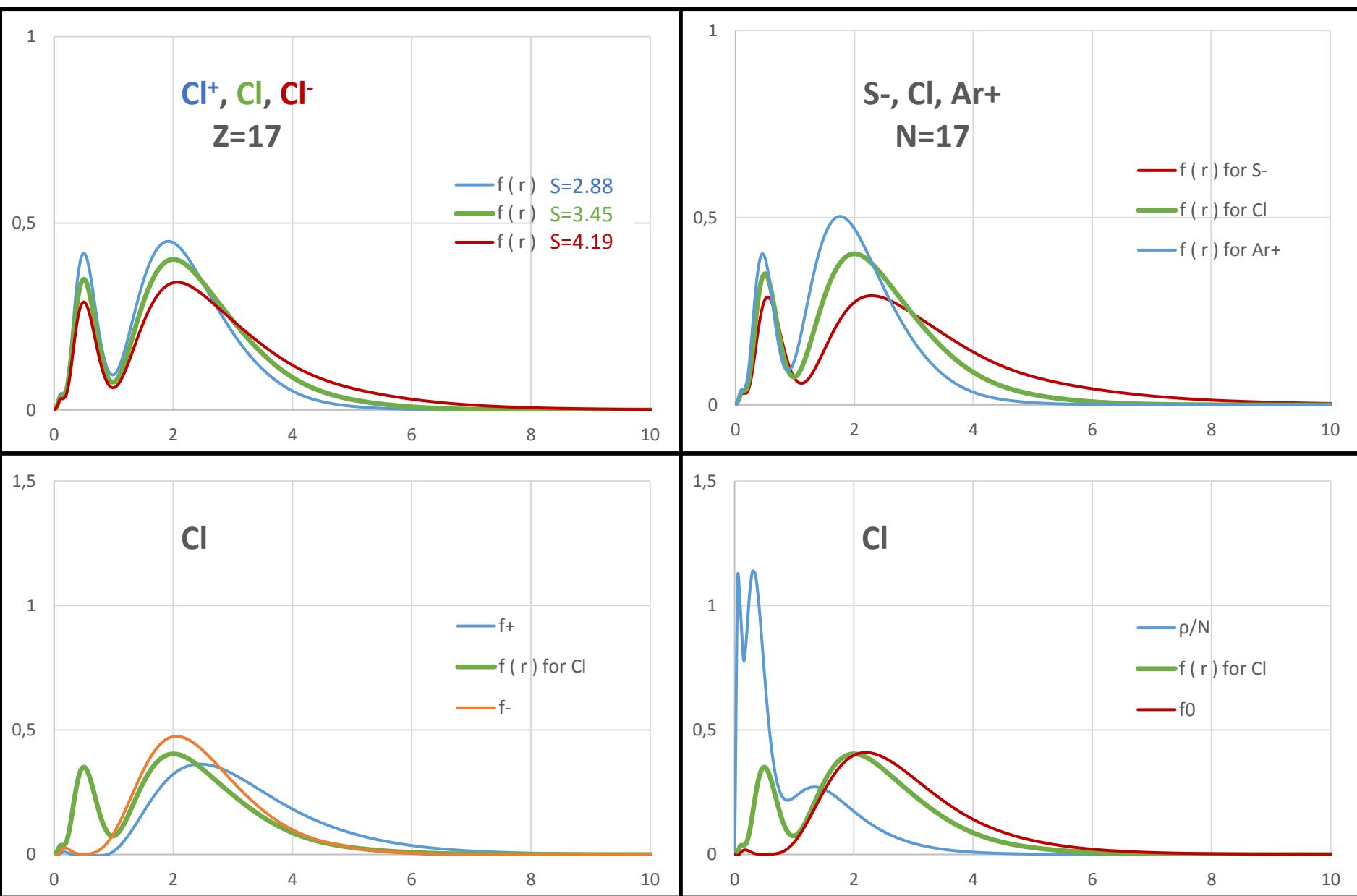
Li	Be		
B	C	N	O
Na	Mg		
K	Ca	Sc	Ti
Al	Si	P	S
Cr	Ge	As	Se
Fe	Co	Ni	Cu
Mo	W	Os	Ru
Re			

Figure S16 Radial distribution for the calculated Fukui functions of S atom, its ions and isoelectronic ions.



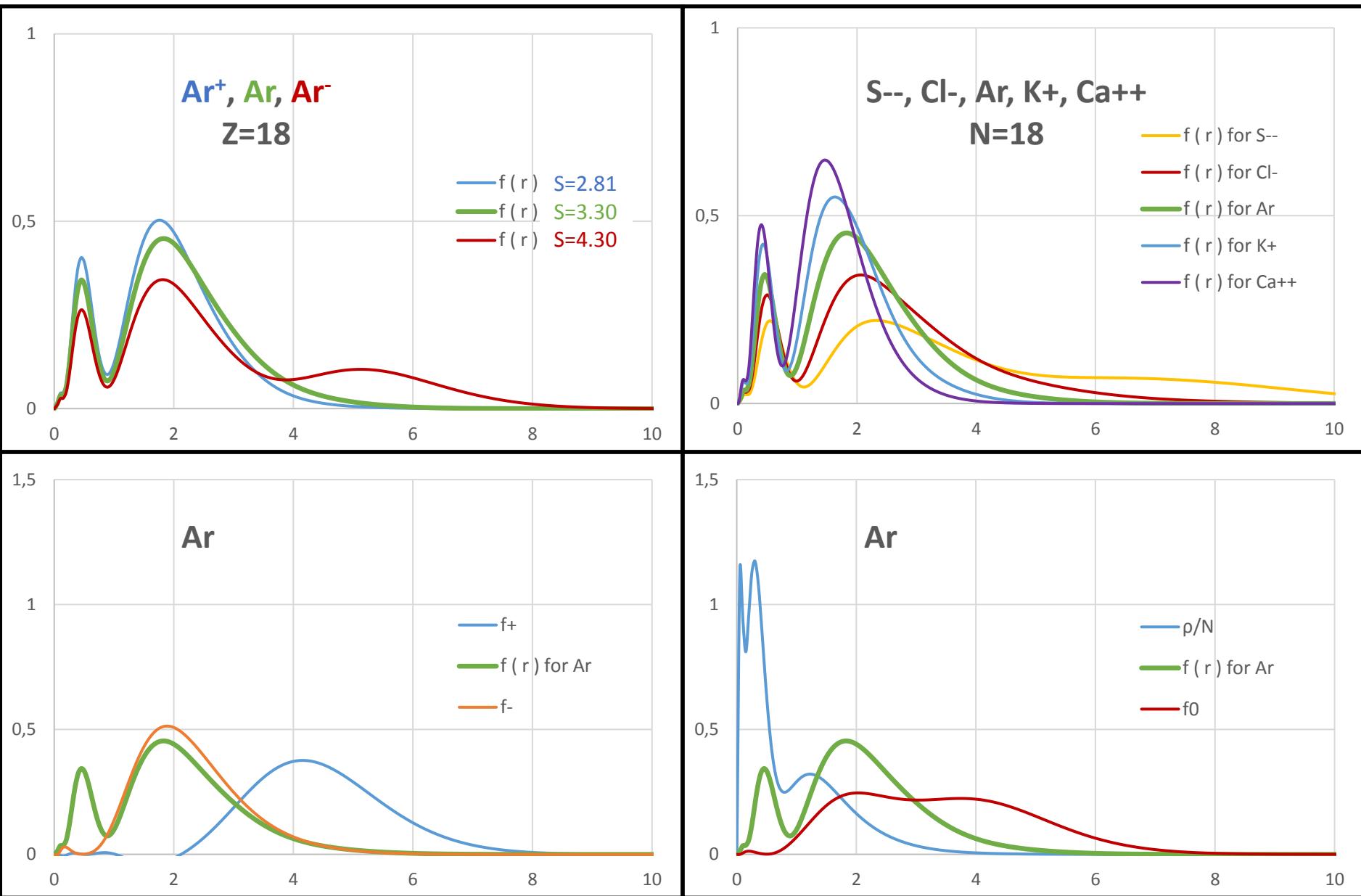
ELEMENTS	
H	He
Li	Be
B	C
N	O
F	Ne
Na	Mg
Al	Si
P	S
Cl	Ar
K	Ca
Sc	Ti
V	Cr
Mn	Fe
Co	Ni
Cu	Zn
Ga	Ge
As	Se
Br	Te
I	Te

**Figure S17 Radial distribution for the calculated Fukui functions of Cl atom, its univalent ions and isoelectronic ions.**



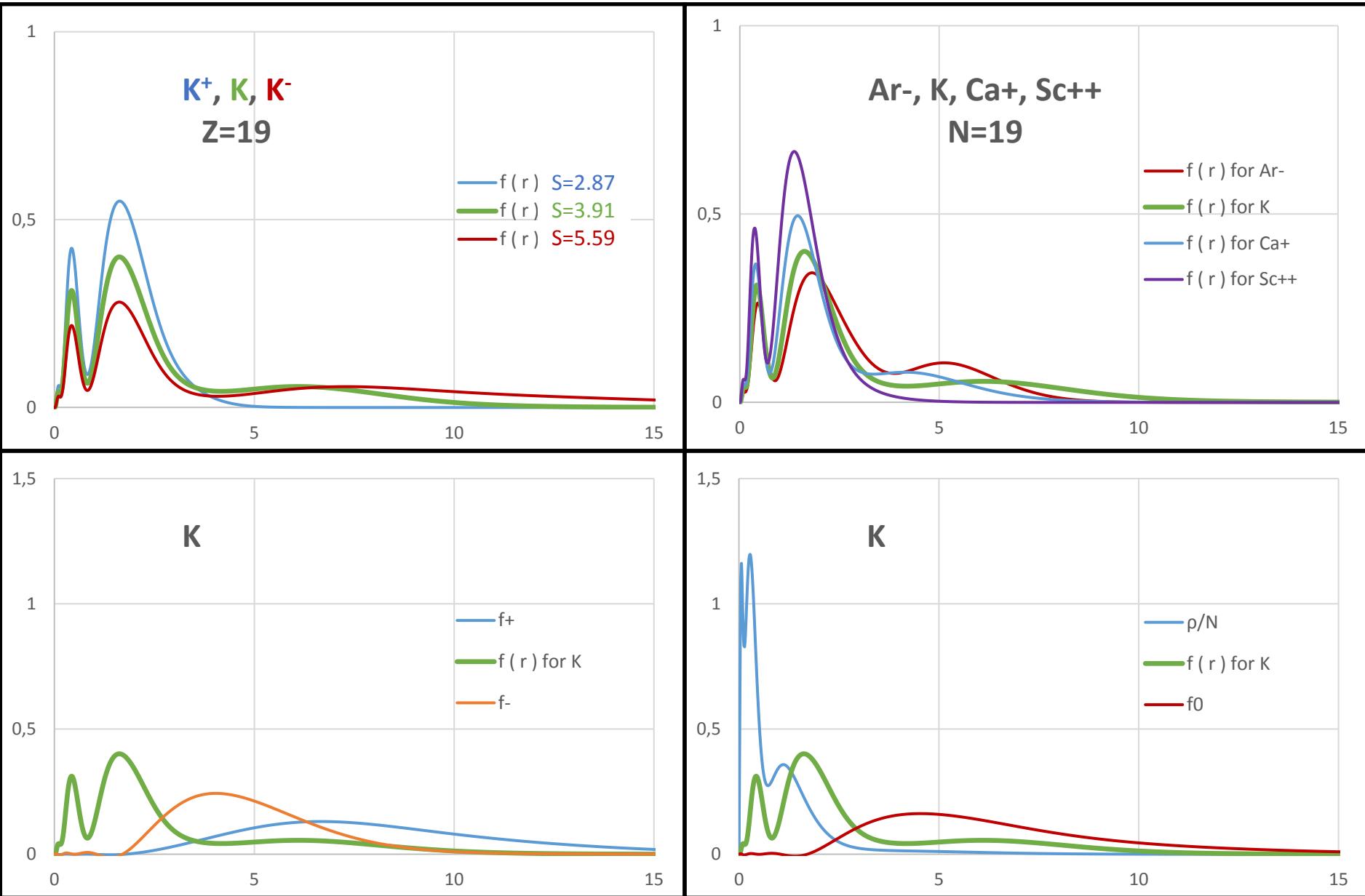
ELEMENTS																	
H	Li	Be	B	C	N	O	F	Ne	Na	Mg	Al	Si	P	S	Cl	Ar	K
Li	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	K

Figure S18 Radial distribution for the calculated Fukui functions of Ar atom, its univalent ions and isoelectronic ions.



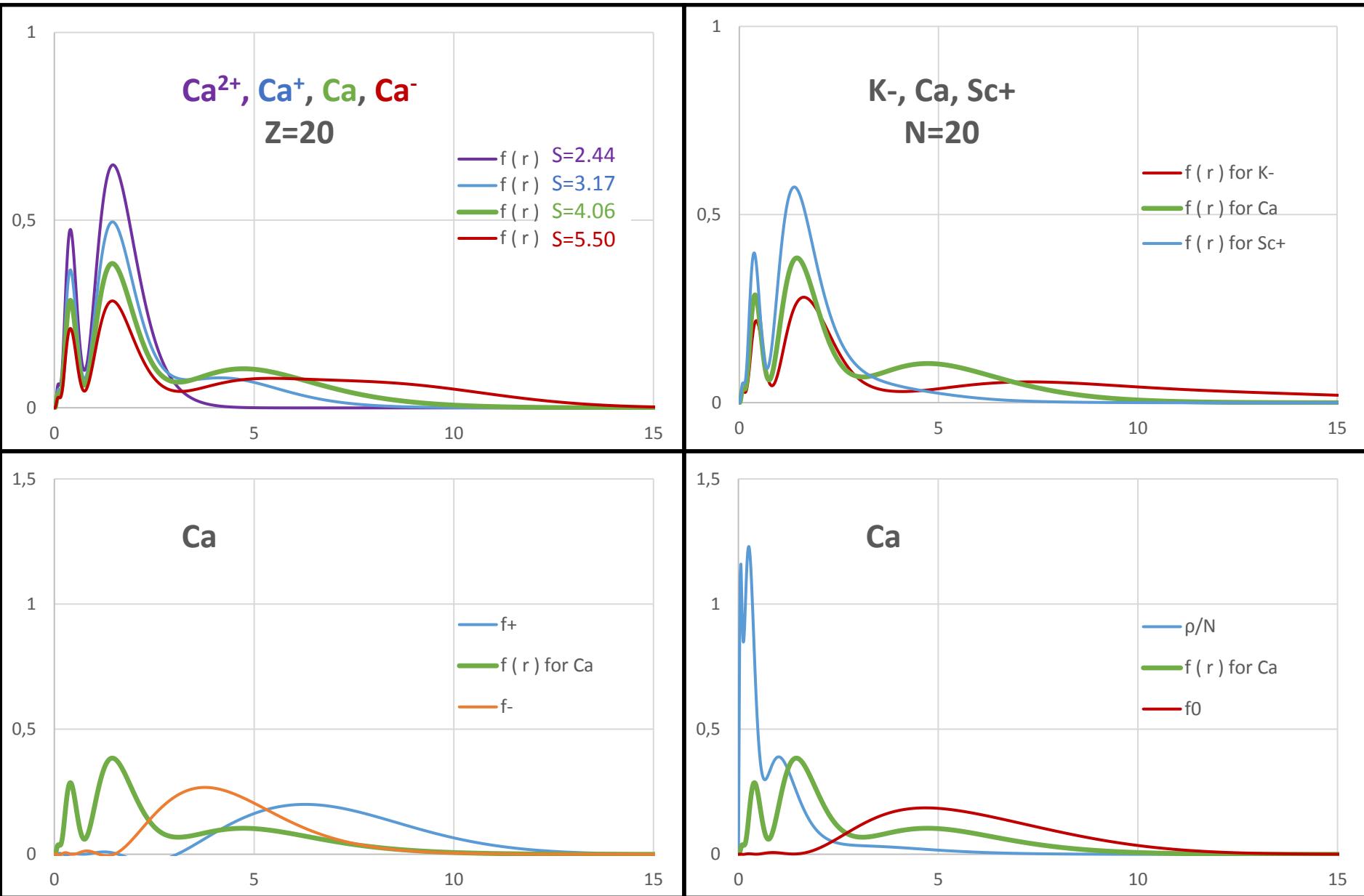
ELEMENTS	
H	He
Li	Be
B	C
N	O
F	Ne
K	Ca
Sc	Ti
V	Cr
Mn	Fe
Co	Ni
Cu	Zn
Ga	Ge
As	P
Sb	Se
Br	Te
I	Te

Figure S19 Radial distribution for the calculated Fukui functions of K atom, its ions and isoelectronic ions.



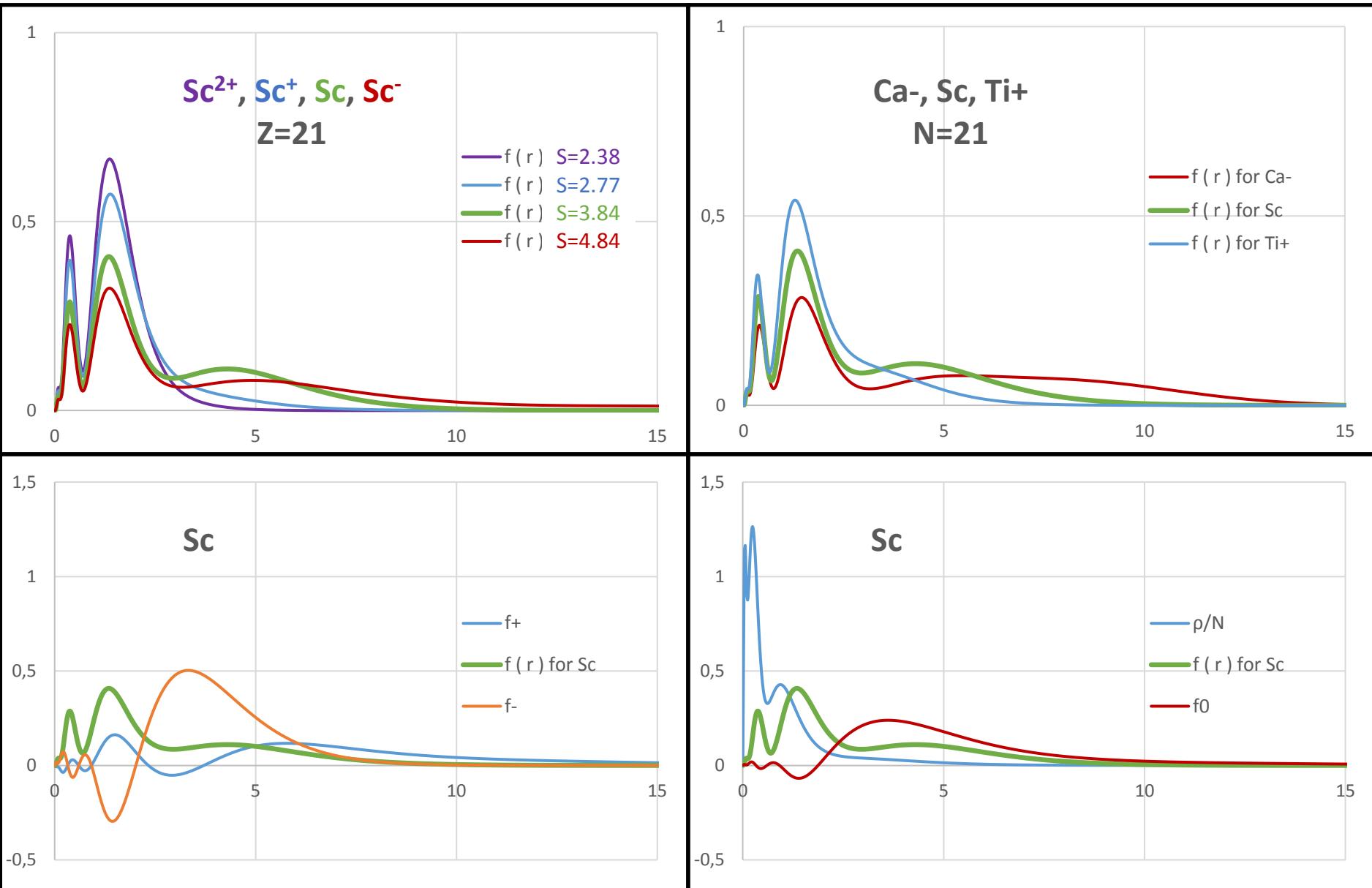
ELEMENTS	
H	He
Li	Be
B	C
C	N
N	O
O	F
F	Ne
Na	Mg
Al	Si
Si	P
P	S
S	Cl
Cl	Ar
K	Ca
Ca	Sc
Sc	Ti
Ti	V
V	Cr
Cr	Mn
Mn	Fe
Fe	Co
Co	Ni
Ni	Cu
Cu	Zn
Zn	Ga
Ga	Ge
Ge	As
As	Se
Se	Br
Br	Kr

Figure S20 Radial distribution for the calculated Fukui functions of Ca atom, its ions and isoelectronic ions.



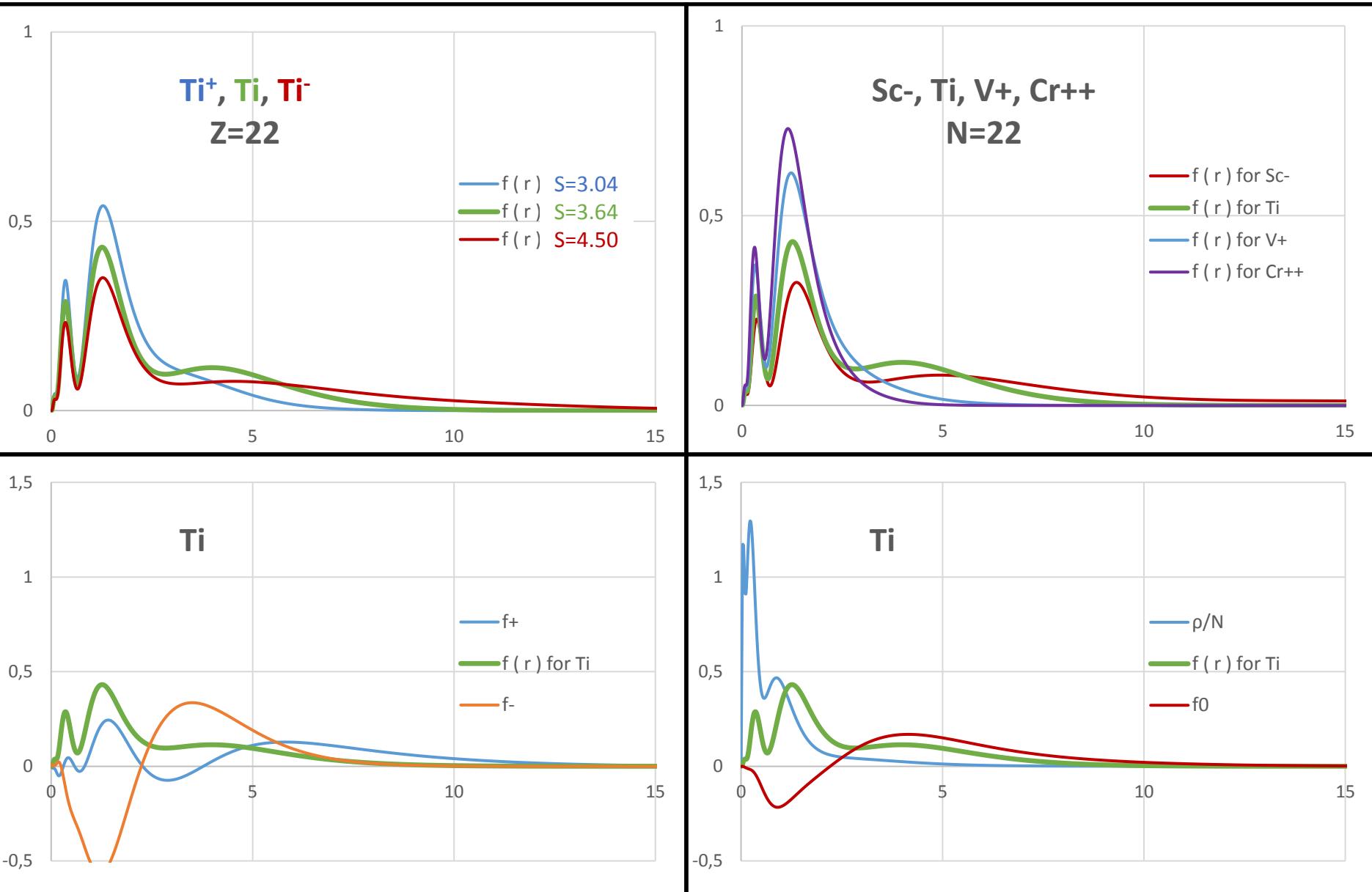
ELEMENTS	
H	He
Li	Be
B	C
C	N
N	O
O	F
F	Ne
Na	Mg
Al	Si
Si	P
P	S
S	Cl
Cl	Ar
K	Ca
Ca	Sc
Sc	Ti
Ti	V
V	Cr
Cr	Mn
Mn	Fe
Fe	Co
Co	Ni
Ni	Cu
Cu	Zn
Zn	Ga
Ga	In
In	Tl
Tl	Br
Br	Kr

**Figure S21** Radial distribution for the calculated Fukui functions of Sc atom, its ions and isoelectronic ions.



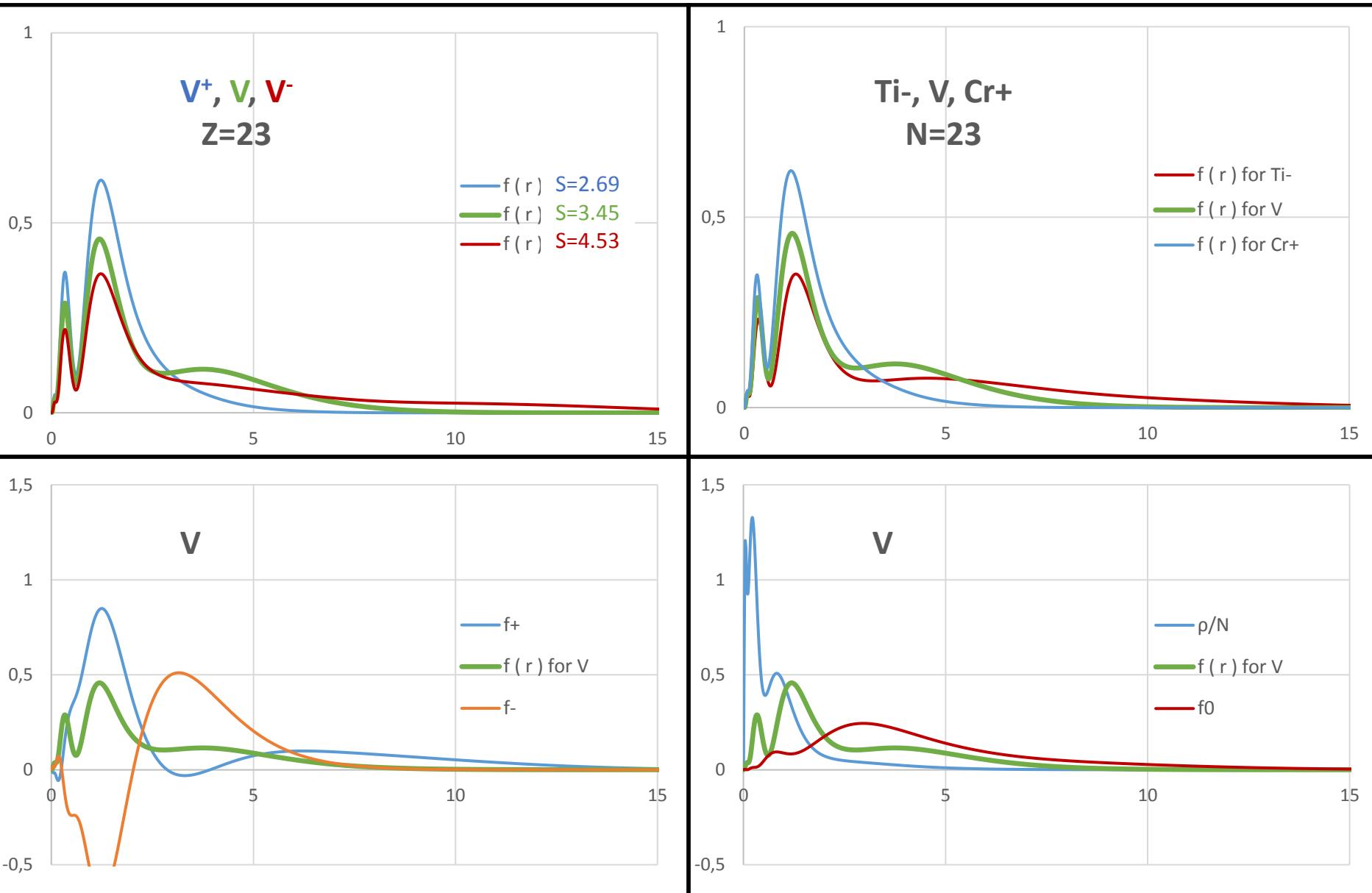
ELEMENTS																	
H	Li	Be	B	C	N	O	F	Ne	Na	Mg	Al	Si	P	S	Cl	Ar	K
Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	

Figure S22 Radial distribution for the calculated Fukui functions of Ti atom, its ions and isoelectronic ions.



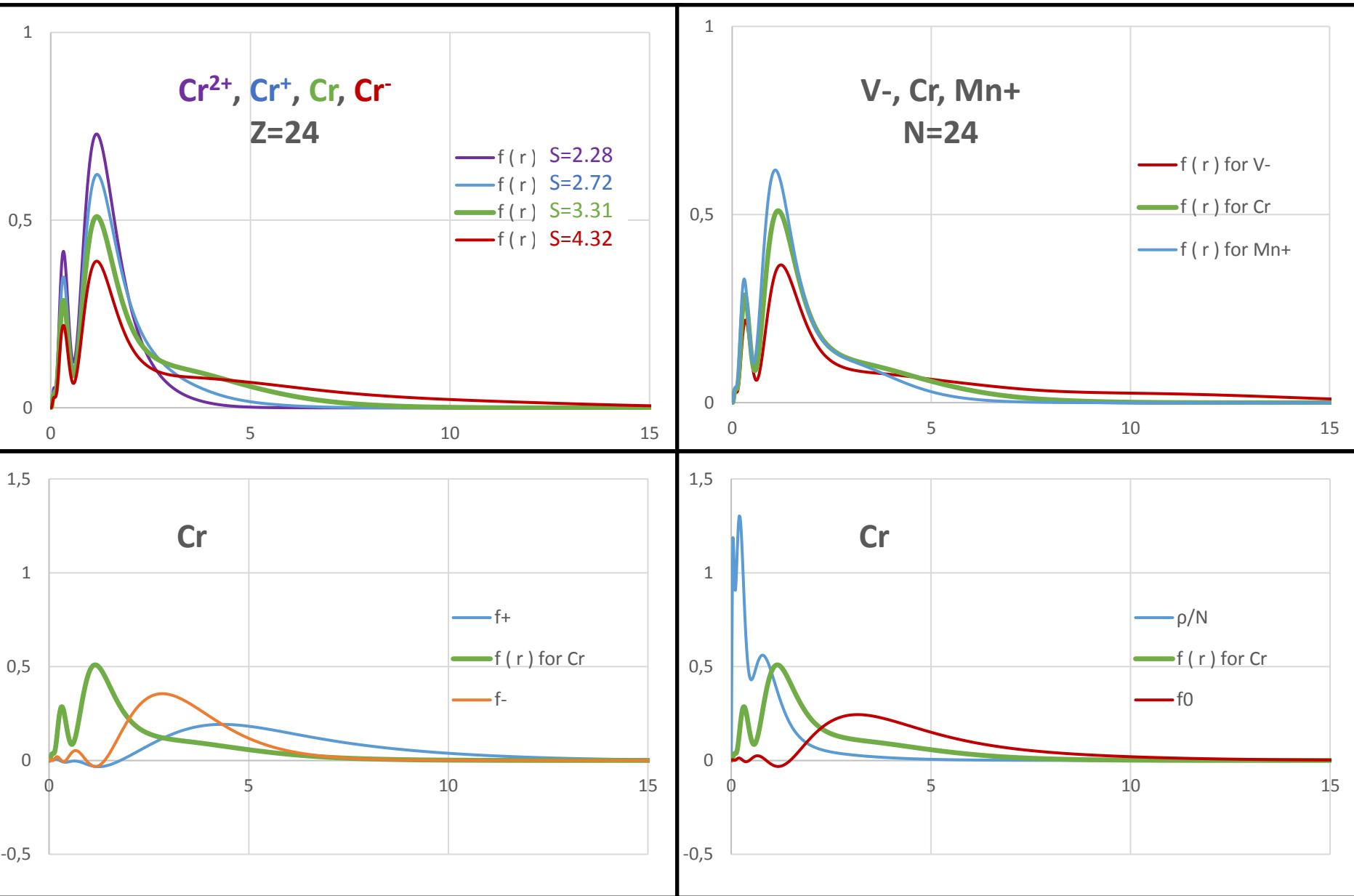
Li	Be		
Na	Mg		
K	Ca	Sc	Ti
Li	Be	V	Cr
Ca	Sc	Cr	Mn
Co	Ni	Mn	Fe
Cr	Co	Fe	Mo
Mn	Cr	Mo	Ti

Figure S23 Radial distribution for the calculated Fukui functions of V atom, its univalent ions and isoelectronic ions.



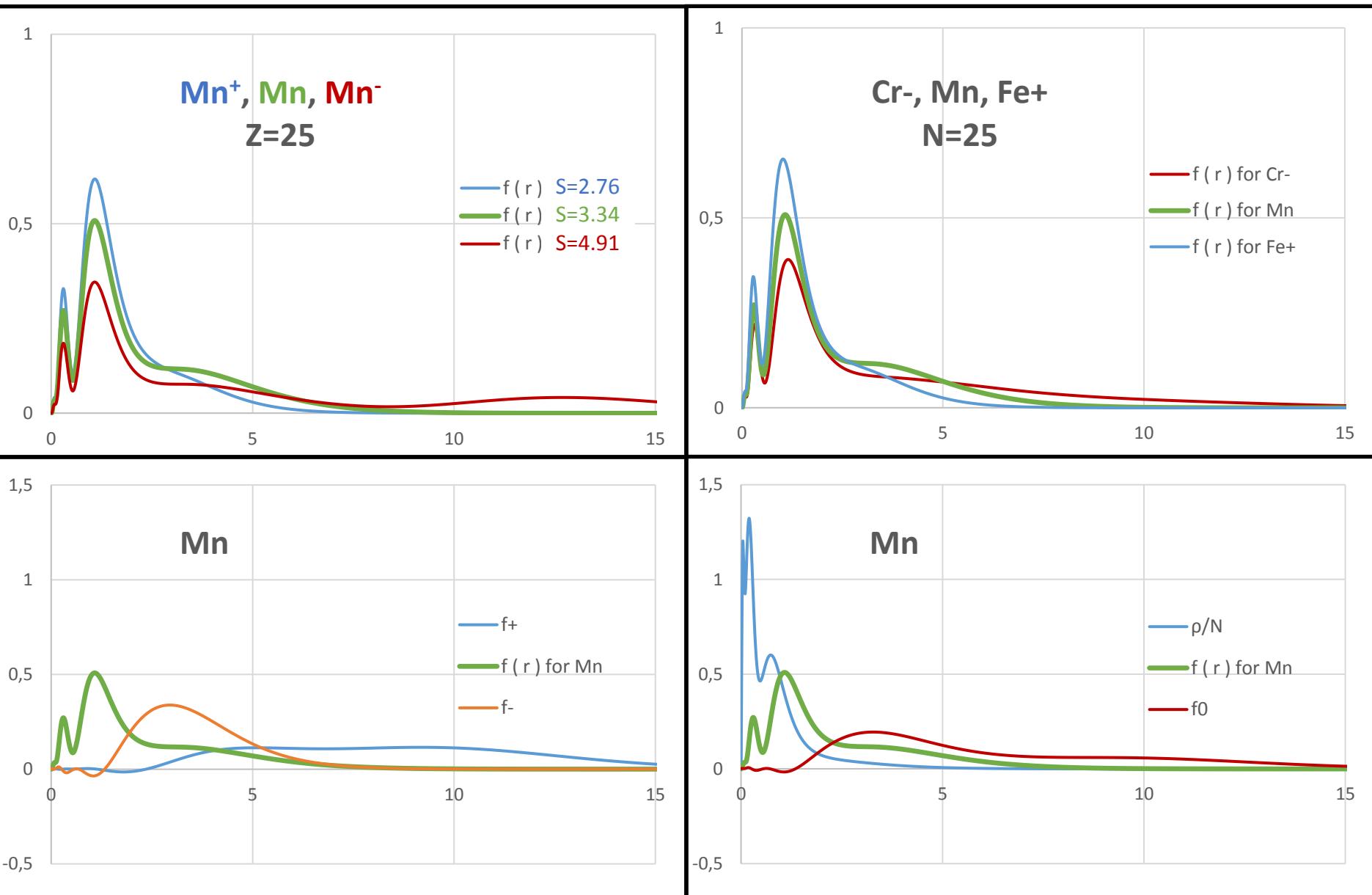
ELEMENTS	
H	He
Li	Be
B	C
N	O
F	Ne
Na	Mg
Al	Si
P	S
Cl	Ar
K	Ca
Sc	Ti
V	Cr
Mn	Fe
Co	Ni
Cu	Zn
Ga	Ge
As	Se
Br	Te
I	Te

Figure S24 Radial distribution for the calculated Fukui functions of Cr atom, its ions and isoelectronic ions.



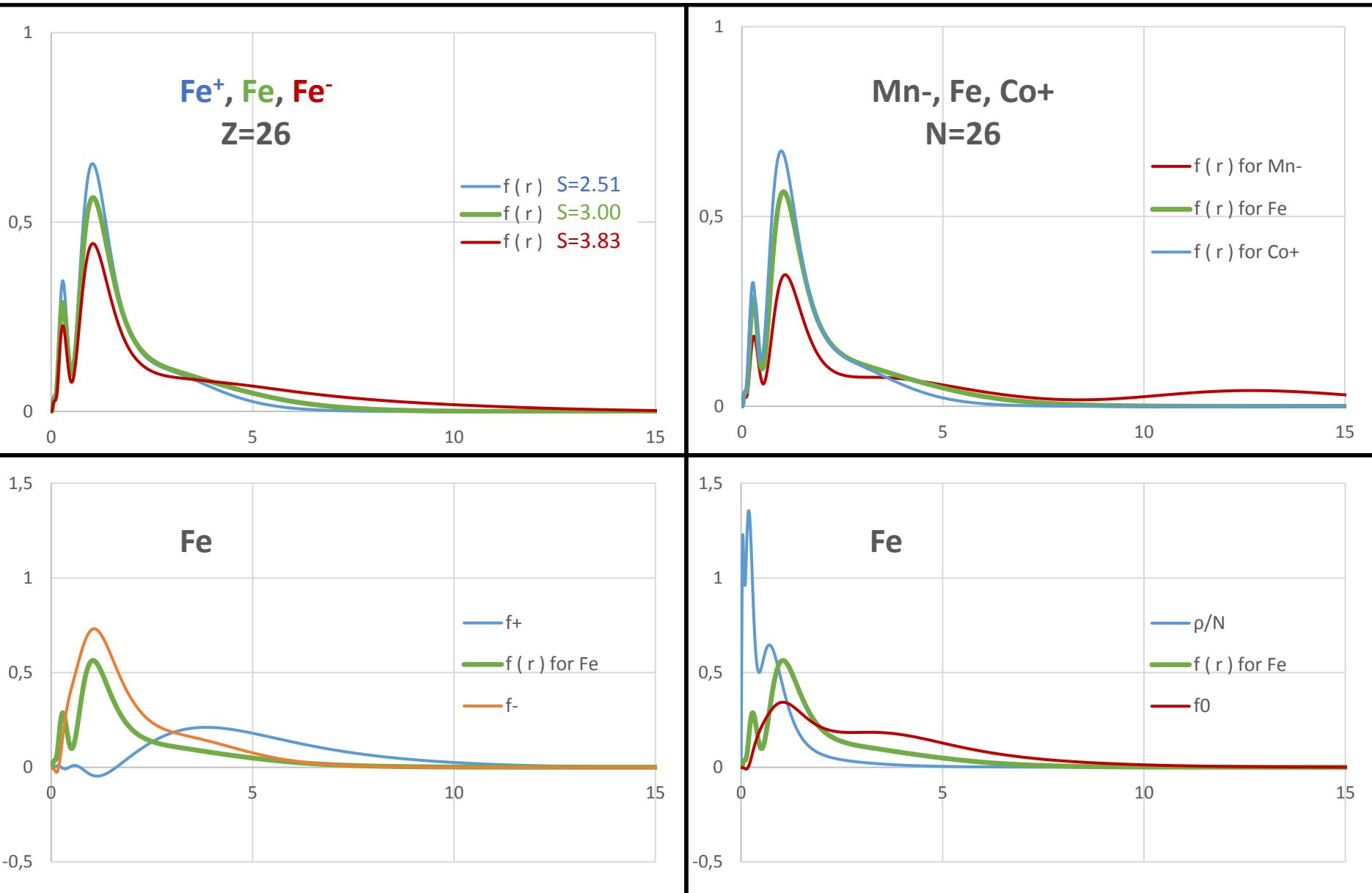
ELEMENTS																	
H	Li	Be	B	C	N	O	F	Ne	Na	Mg	Al	Si	P	S	Cl	Ar	K
Li	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	K

Figure S25 Radial distribution for the calculated Fukui function of Mn atom, its univalent ions and isoelectronic ions.



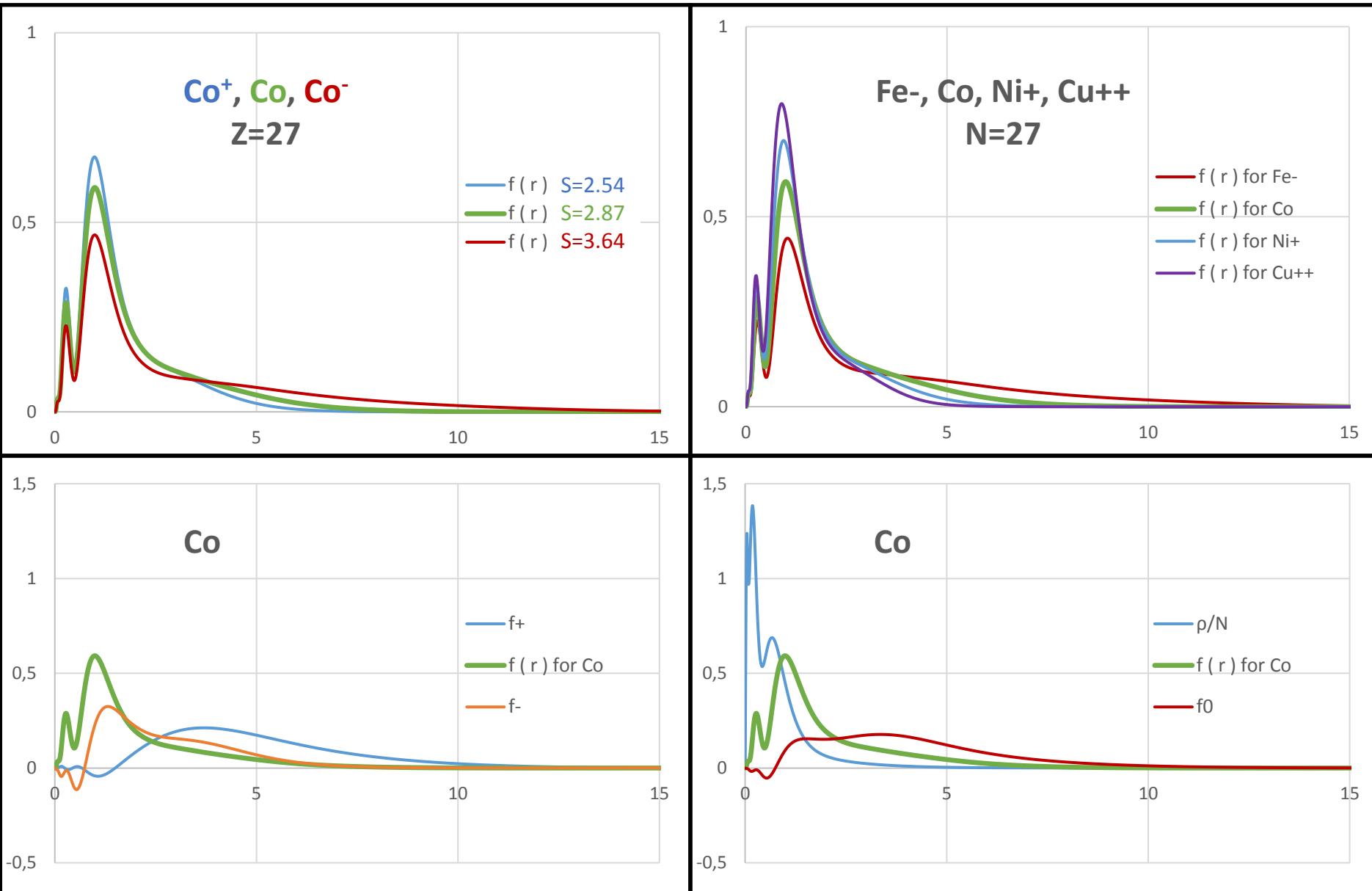
ELEMENTS	
H	He
Li	Be
B	C
N	O
F	Ne
K	Ca
Sc	Ti
V	Cr
Mn	Fe
Co	Ni
Zn	Cu
Ga	Ge
As	P
Sb	Se
Br	Te
I	Te

Figure S26 Radial distribution for the calculated Fukui functions of Fe atom, its univalent ions and isoelectronic ions.



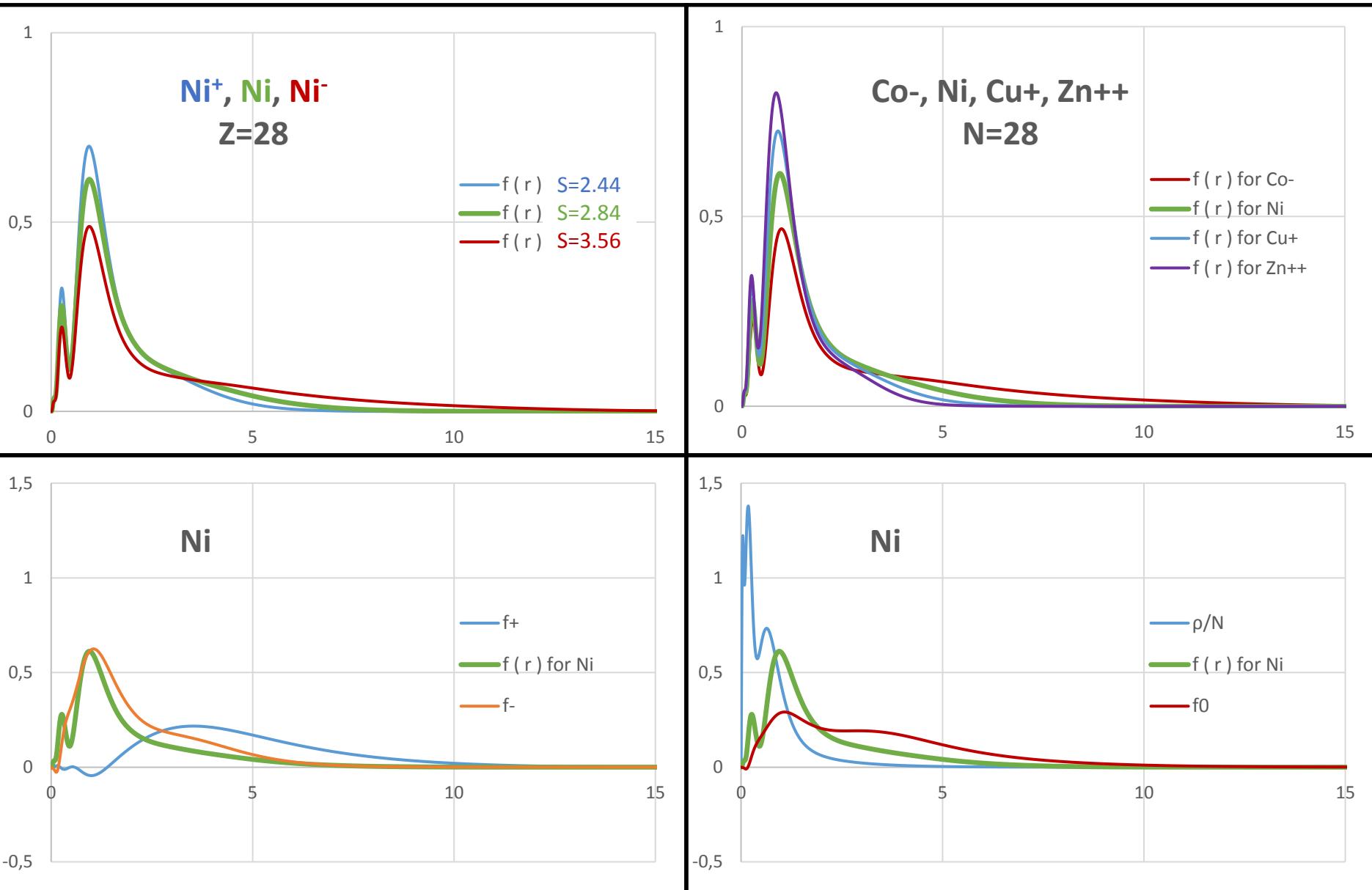
ELEMENTS	
H	He
Li	Be
B	C
N	O
F	Ne
Na	Mg
K	Ca
Sc	Ti
V	Cr
Mn	Fe
Co	Ni
Cu	Zn
Ga	Ge
As	P
Sb	Se
Br	Te
I	Te

Figure S27 Radial distribution for the calculated Fukui functions of Co atom, its ions and isoelectronic ions.



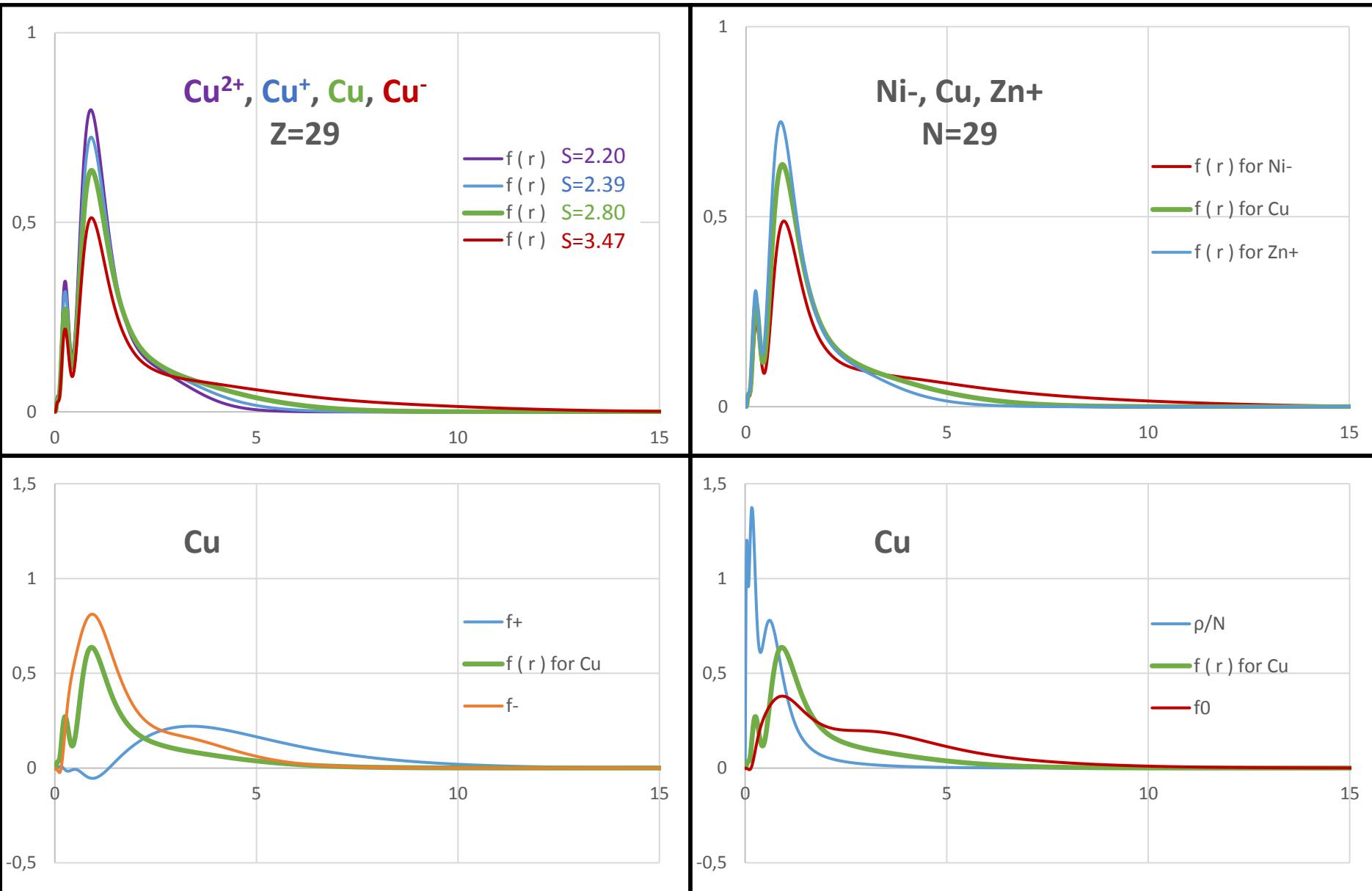
ELEMENTS																	
H	Li	Be	B	C	N	O	F	Ne									
He	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	P	S	Cl

Figure S28 Radial distribution for the calculated Fukui functions of Ni atom, its ions and isoelectronic ions.



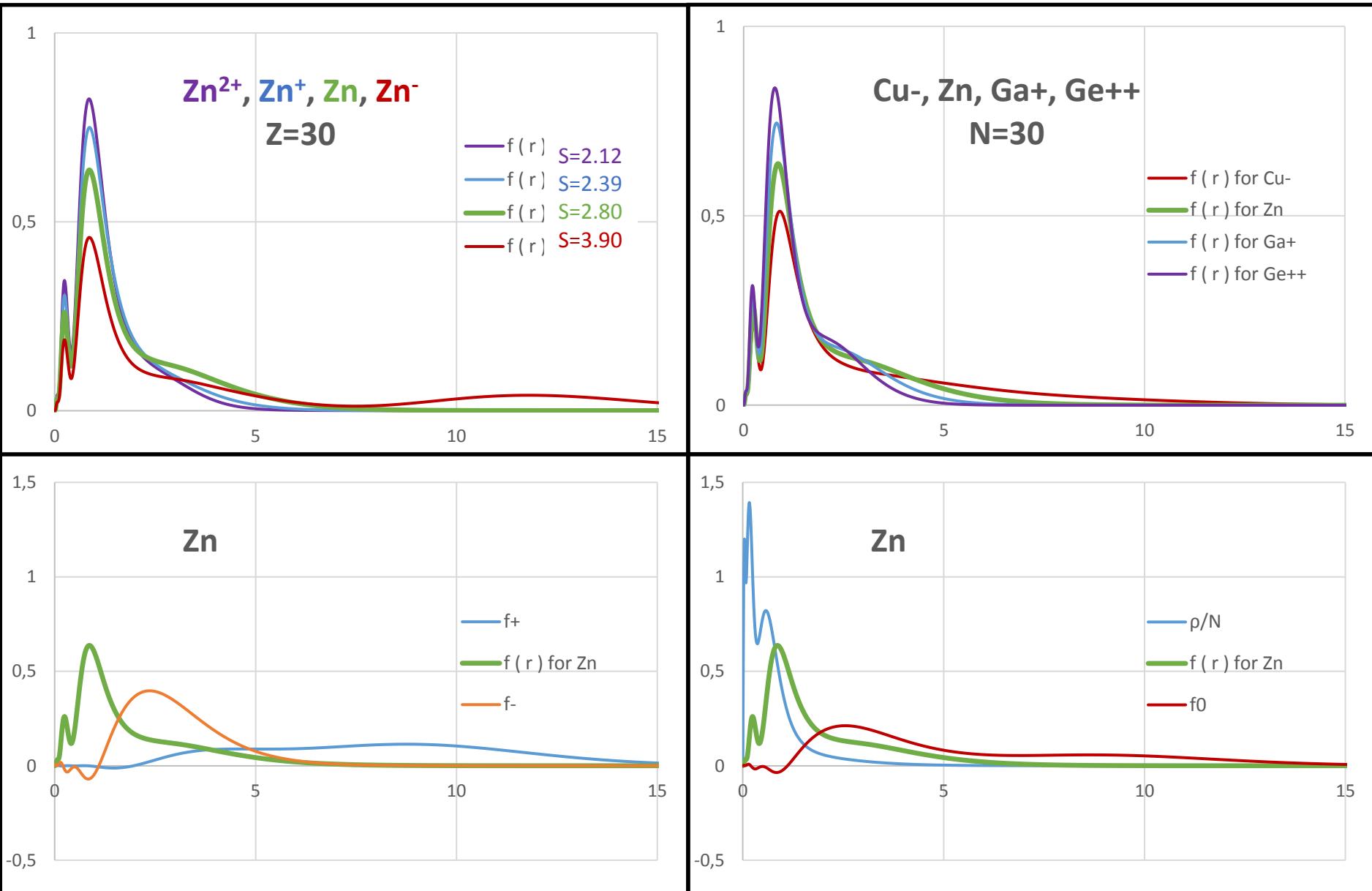
ELEMENTS																	
H	He	B	C	N	O	F	Ne	Na	Mg	Al	Si	P	S	Cl	Ar	K	Ca
Li	Be	Ti	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	Fr	Rb

Figure S29 Radial distribution for the calculated Fukui functions of Cu atom, its ions and isoelectronic ions.



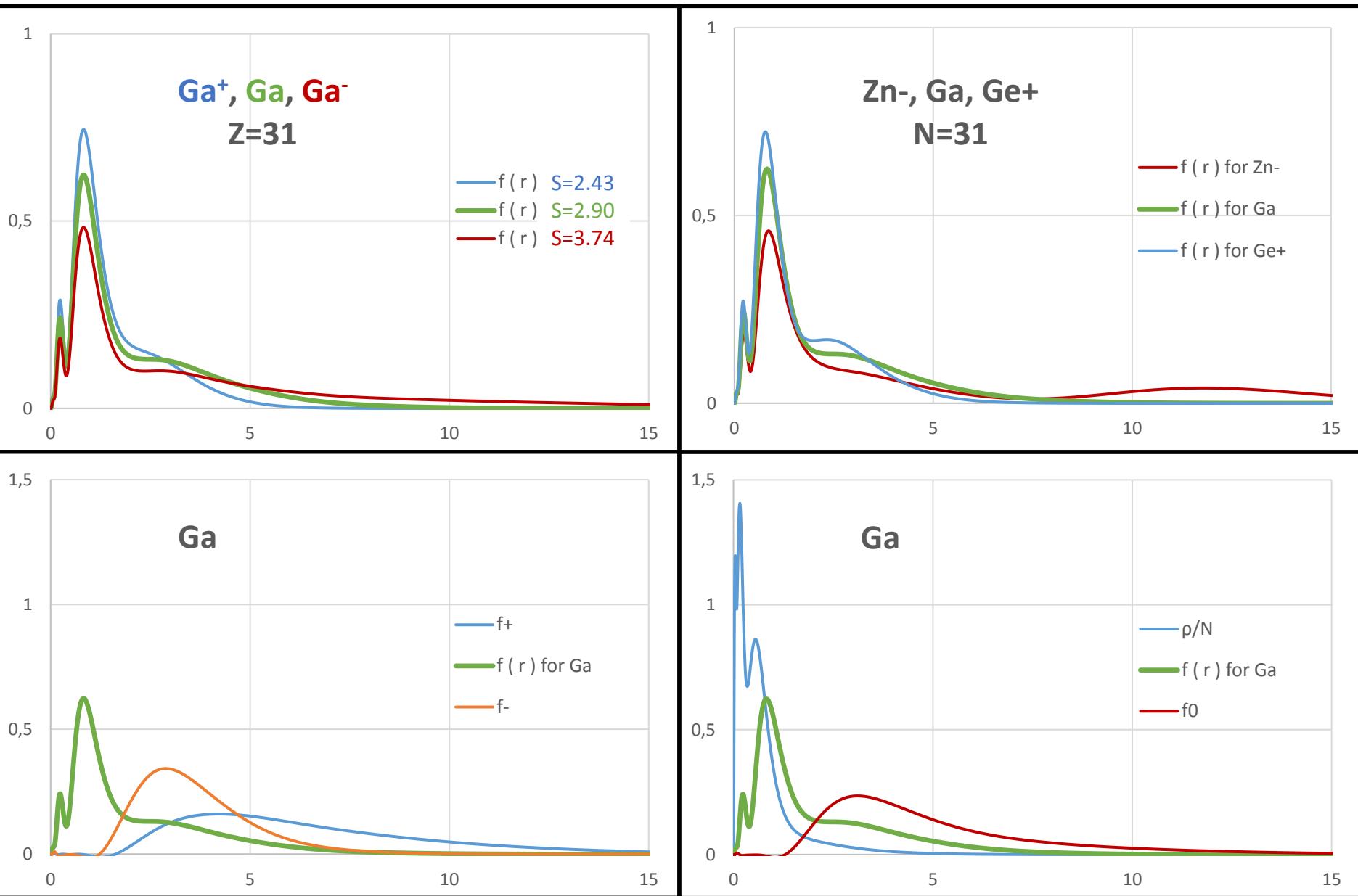
H	He										
Li	Be										
B	C	N	O	F							
N	Ca	Si	P	S	Cl						
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
Mg	Al	Si	P	S	Cl	Ca	Sr	Ba	Sr	Br	K

Figure S30 Radial distribution for the calculated Fukui functions of Zn atom, its ions and isoelectronic ions.



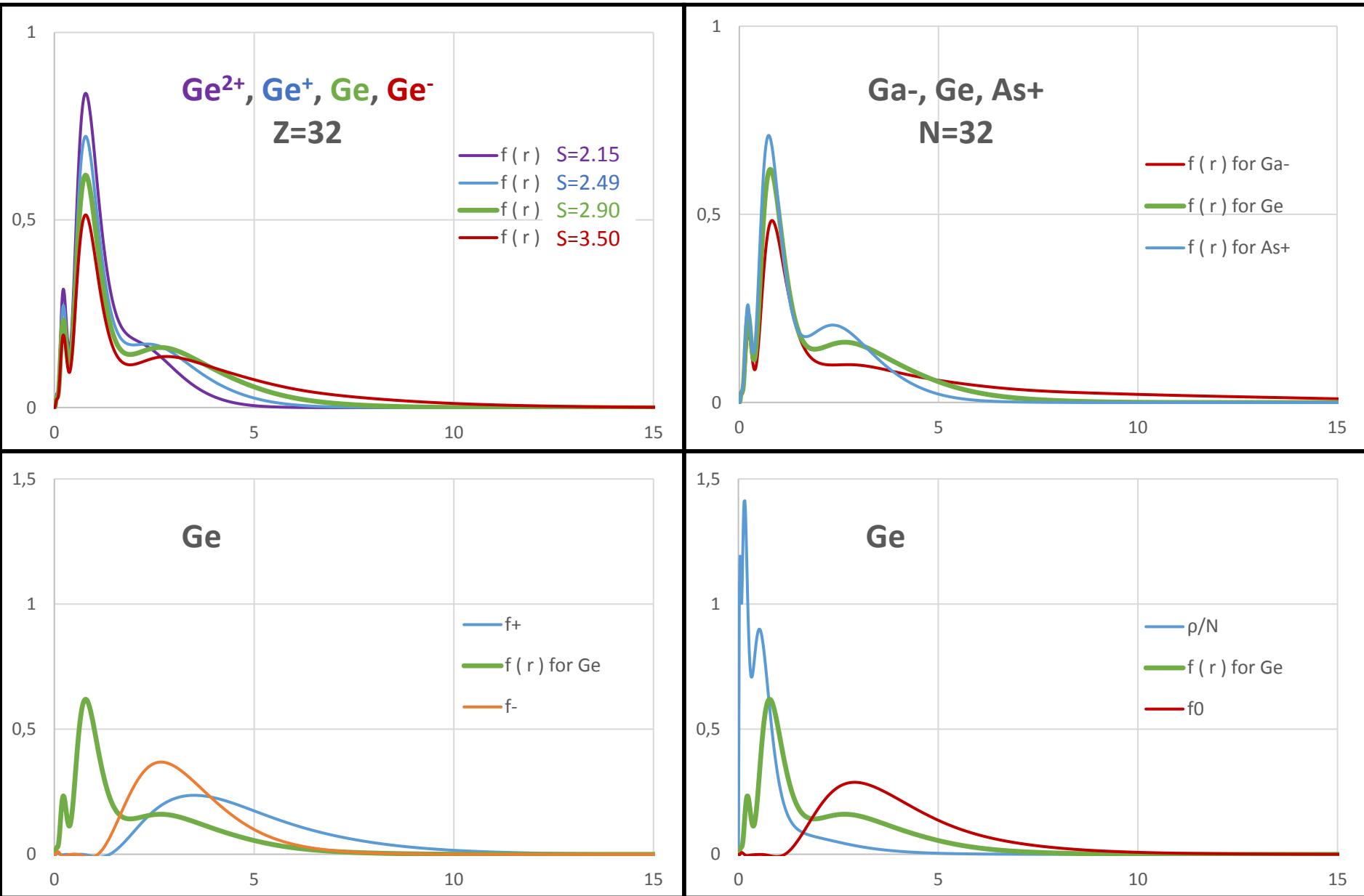
ELEMENTS																	
H	Li	Be	B	C	N	O	F	Ne	Na	Mg	Al	Si	P	S	Cl	Ar	K
Li	Ca	Sc	Ti	Zr	Hf	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	Rb	

Figure S31 Radial distribution for the calculated Fukui functions of Ga atom, its univalent ions and isoelectronic ions.



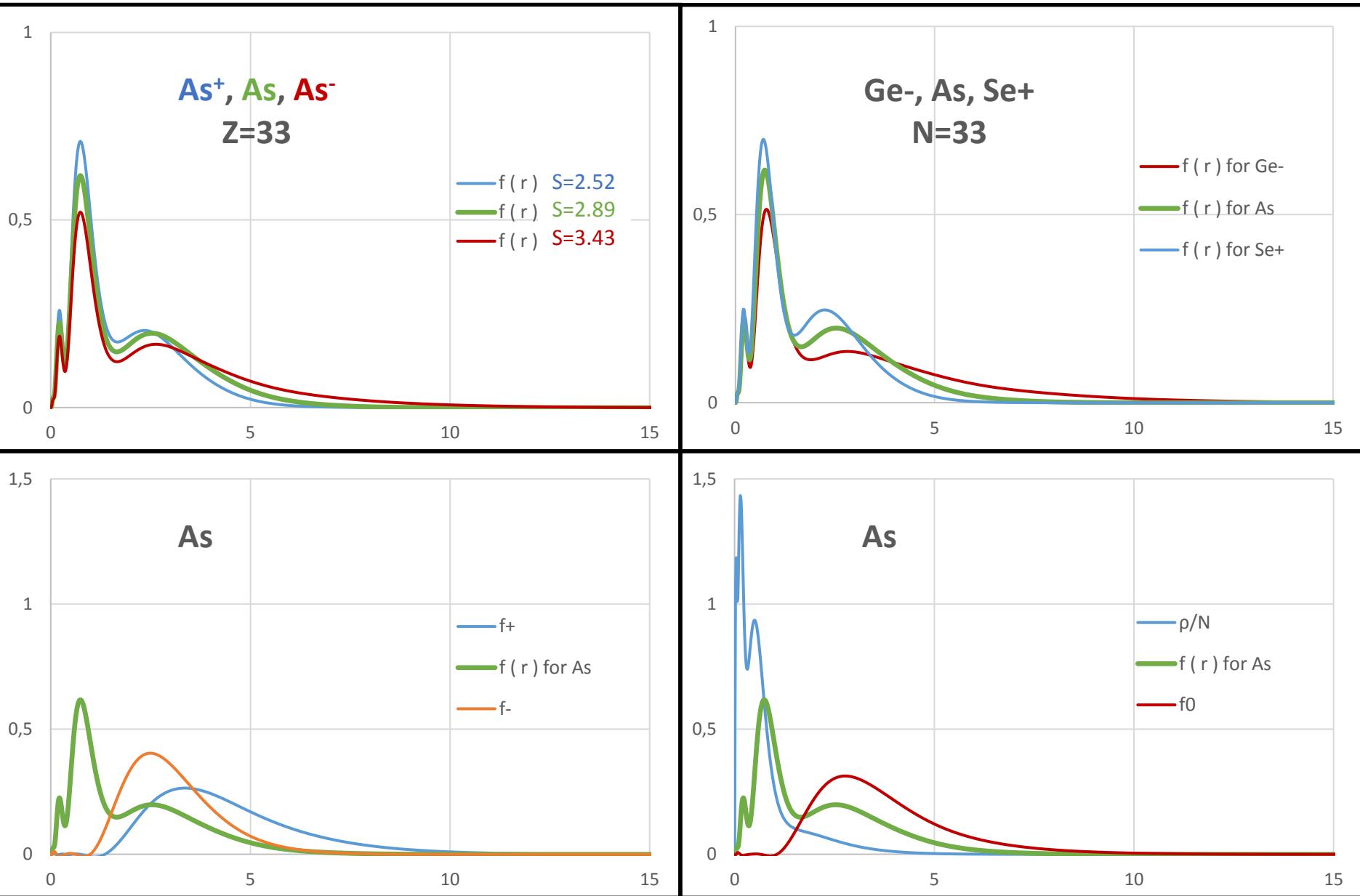
ELEMENTS	
H	He
Li	Be
B	C
C	N
N	O
O	F
F	Ne
Na	Mg
Al	Si
P	S
S	Cl
Cl	Ar
K	Ca
Sc	Ti
V	Cr
Cr	Mn
Mn	Fe
Co	Ni
Ni	Cu
Cu	Zn
Zn	As
As	Pb
Pb	Br
Br	Kr

Figure S32 Radial distribution for the calculated Fukui functions of Ge atom, its ions and isoelectronic ions.



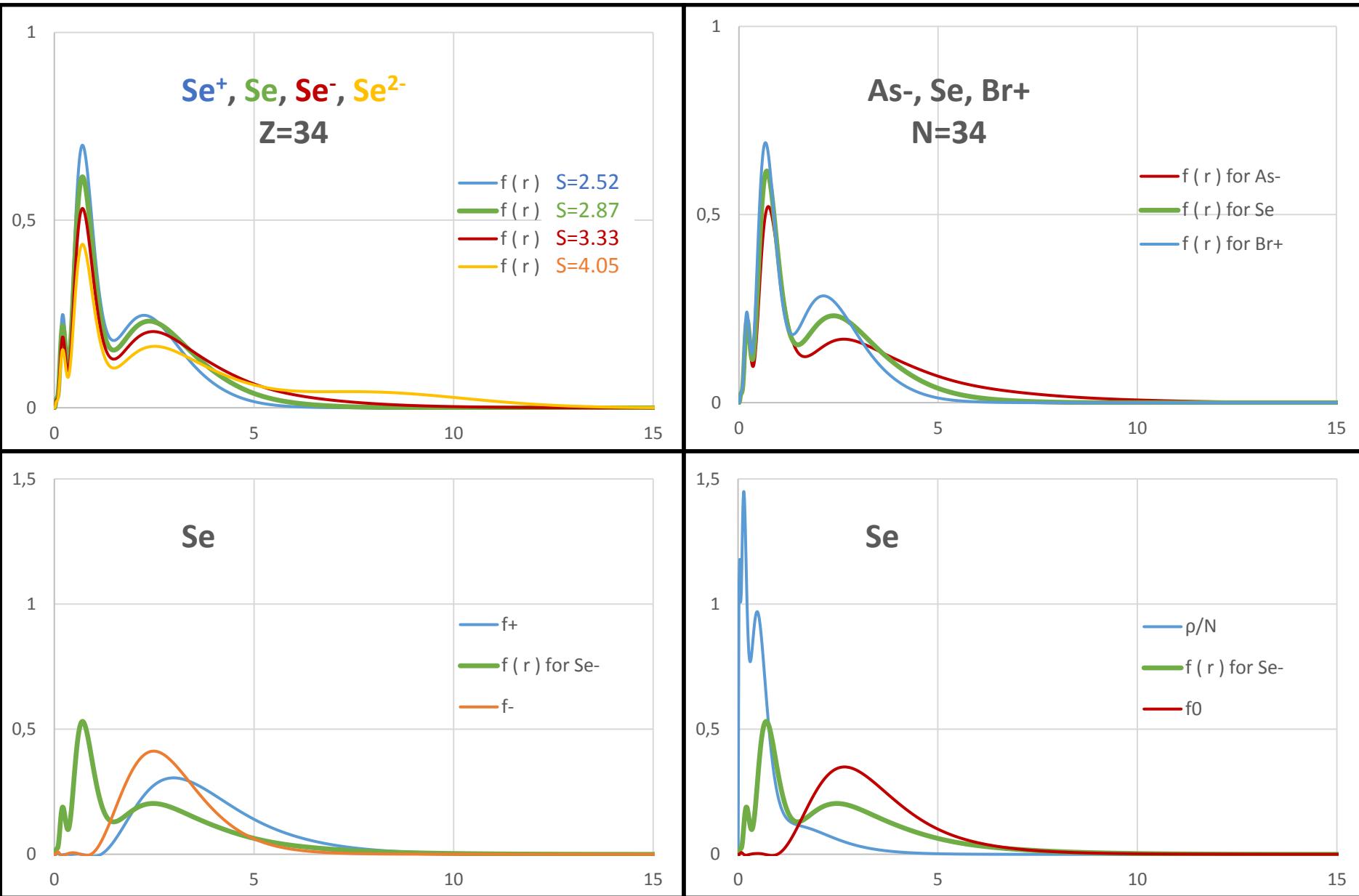
ELEMENTS	
H	He
Li	Be
B	C
N	O
F	Ne
Na	Mg
K	Ca
Sc	Ti
V	Cr
Mn	Fe
Co	Ni
Cu	Zn
Ga	Ge
As	P
Sb	Te
Bi	I

Figure S33 Radial distribution for the calculated Fukui functions of As atom, its univalent ions and isoelectronic ions.



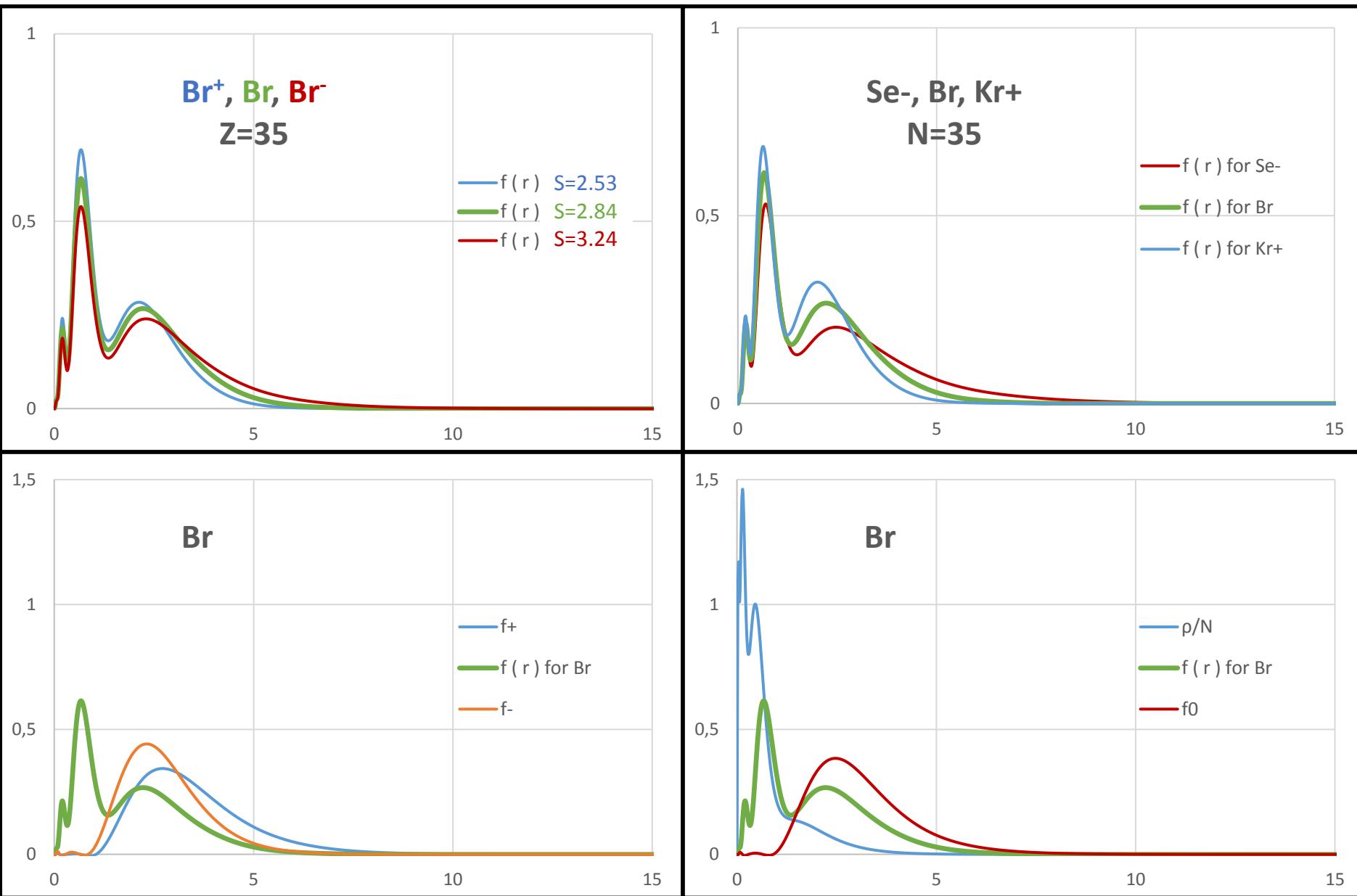
ELEMENTS	
H	He
Li	Be
B	C
C	N
O	F
N	Ne
P	Na
Al	Mg
Si	Ca
Si	Sc
P	Ti
Ca	V
Sc	Cr
Al	Mn
Ca	Co
Sc	Ni
Al	Cu
Ca	Zn
Sc	As
Al	Br
Ca	K

Figure S34 Radial distribution for the calculated Fukui functions of Se atom, its ions and isoelectronic ions.



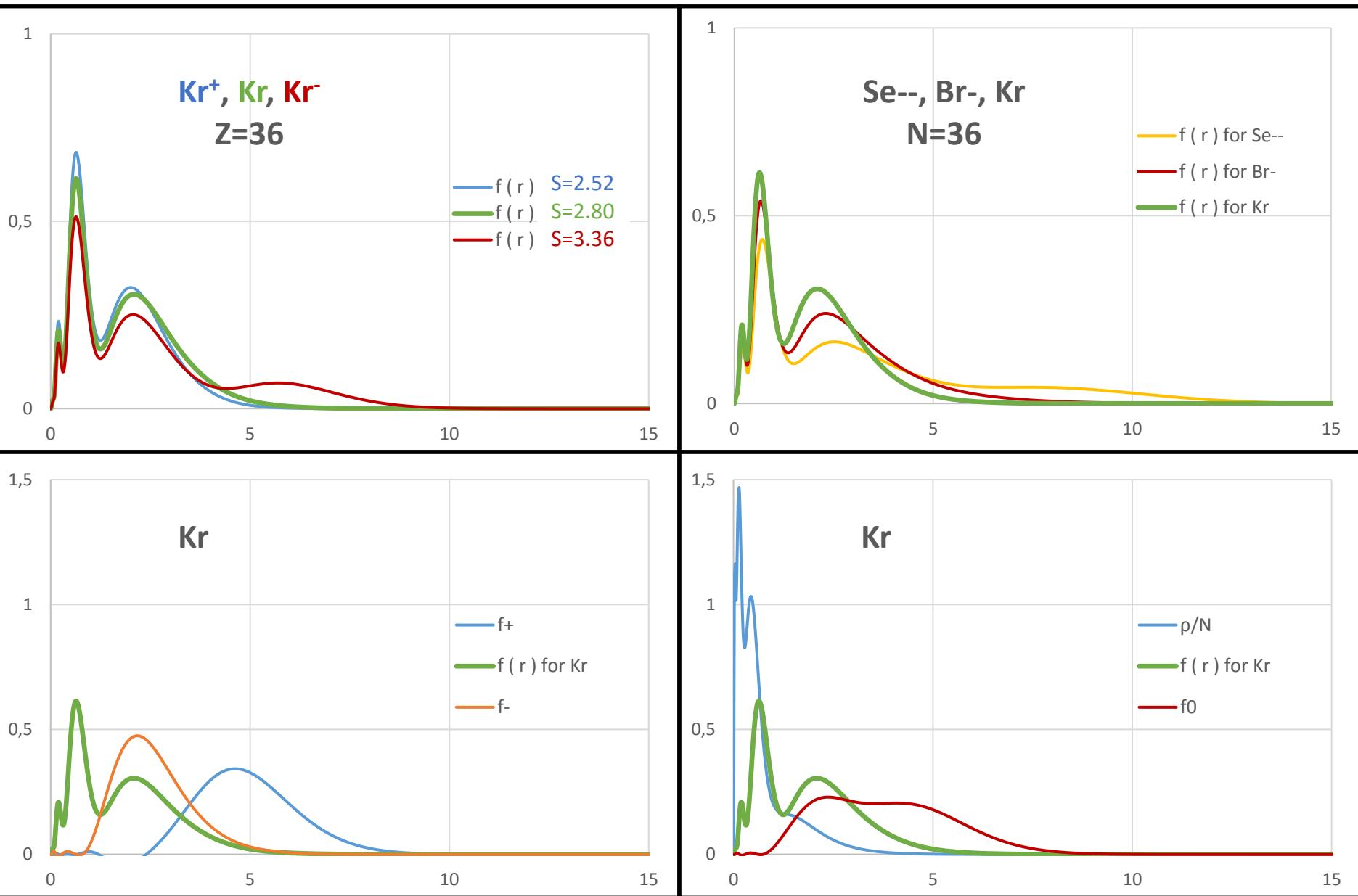
ELEMENTS	
H	He
Li	Be
B	C
N	O
F	Ne
K	Ca
Si	P
Al	S
Cl	Ar
Mg	Ca
Na	Sc
Cr	Ti
Fe	V
Co	Cr
Ni	Mn
Cu	Fe
Zn	Co
Ge	As
Se	Br
Te	I
At	Te
Bi	At

Figure S35 Radial distribution for the calculated Fukui functions of Br atom, its univalent ions and isoelectronic ions.



ELEMENTS	
H	He
Li	Be
B	C
N	O
F	Ne
Na	Mg
Al	Si
P	S
Cl	Ar
K	Ca
Sc	Ti
V	Cr
Cr	Mn
Fe	Co
Ni	Cu
Zn	Ge
Ga	As
In	Se
Tl	Br
Pb	I

Figure S36 Radial distribution for the calculated Fukui functions of Kr atom, its univalent ions and isoelectronic ions.



ELEMENTS																	
H	Li	Be	B	C	N	O	F	Ne	Na	Mg	Al	Si	P	S	Cl	Ar	K
Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr	Rb