Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting Information - Can we talk about ionic bonds in molecules? Yes, just as we do for covalent bonds

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Table S1: Occupations of the three highest occupied NOs in different states of LiH, at different R(Li-H) (Å) distances.

	$1\ ^1\Sigma$			$2\ ^1\Sigma$			$3\ ^1\Sigma$		
R	ϕ_1	ϕ_2	ϕ_3	ϕ_1	ϕ_2	ϕ_3	ϕ_1	ϕ_2	ϕ_3
2.00	1.99992	1.93251	0.05042	1.99987	0.99926	0.99921	1.99990	0.99926	0.99921
4.00	1.99992	1.37860	0.62066	1.99992	1.72964	0.26694	1.99992	1.81401	0.17930
8.00	1.99991	1.00480	0.99514	1.99990	1.03941	0.96054	1.99996	1.96718	0.02649

Table S2: QTAIM atomic charges for different states of LiH, at different R(Li-H) (Å) distances.

	$1\ ^1\Sigma$		$2\ ^1\Sigma$		$3\ ^1\Sigma$	
R	H	Li	H	Li	H	Li
2.00	-0.8950	0.8950	-0.0167	0.0169	-0.0836	0.0840
4.00	-0.0830	0.0831	-0.5119	0.5111	-0.5028	0.5015
8.00	-0.0001	0.0002	-0.0018	-0.0163	-0.8918	0.8260

Figure S1: Isocontours (blue, positive; red, negative) of $\nabla^2\rho$ for the aug-cc-pVDZ/FCI $1^1\Sigma$ (top) and $2^1\Sigma$ (bottom) states of LiH at $R = 2.0$ Å.

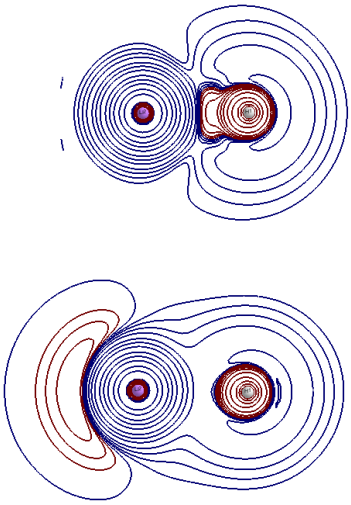

Figure S2: Three highest occupied NOs (ϕ_1,ϕ_2,ϕ_3) for the $1^1\Sigma$ R(Li-H)=2.0 Å geometry. $|\phi| = 0.08$.

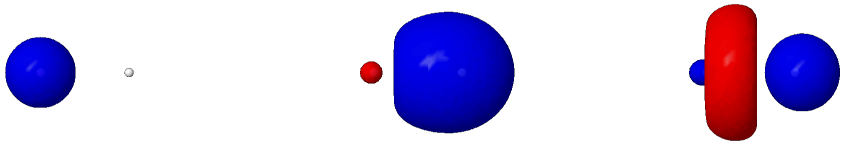

Figure S3: Three highest occupied NOs (ϕ_1,ϕ_2,ϕ_3) for the $2^1\Sigma$ R(Li-H)=2.0 Å geometry. $|\phi| = 0.08$.

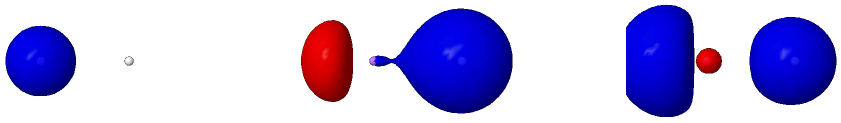

Figure S4: Three highest occupied NOs (ϕ_1,ϕ_2,ϕ_3) for the $3^1\Sigma$ R(Li-H)=2.0 Å geometry. $|\phi| = 0.08$.

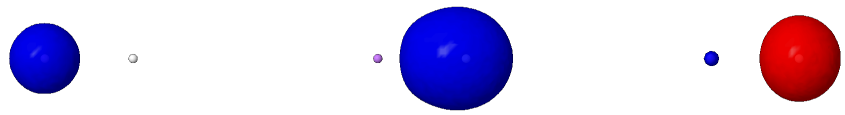

Figure S5: Three highest occupied NOs (ϕ_1,ϕ_2,ϕ_3) for the $1^1\Sigma$ R(Li-H)=4.0 Å geometry. $|\phi| = 0.08$.

Figure S6: Three highest occupied NOs (ϕ_1,ϕ_2,ϕ_3) for the $2^1\Sigma$ R(Li-H)=4.0 Å geometry. $|\phi| = 0.08$.

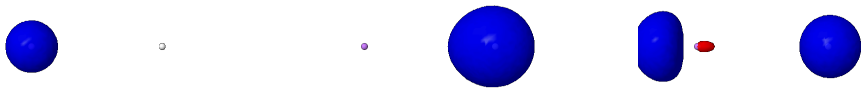

Figure S7: Three highest occupied NOs (ϕ_1,ϕ_2,ϕ_3) for the $3^1\Sigma$ R(Li-H)=4.0 Å geometry. $|\phi| = 0.08$.

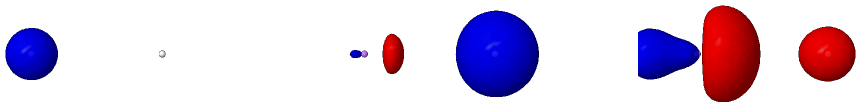

Figure S8: Three highest occupied NOs (ϕ_1,ϕ_2,ϕ_3) for the $1^1\Sigma$ R(Li-H)=8.0 Å geometry. $|\phi| = 0.08$.

Figure S9: Three highest occupied NOs (ϕ_1,ϕ_2,ϕ_3) for the $2^1\Sigma$ R(Li-H)=8.0 Å geometry. $|\phi| = 0.08$.

Figure S10: Three highest occupied NOs (ϕ_1,ϕ_2,ϕ_3) for the $3^1\Sigma$ R(Li-H)=8.0 Å geometry. $|\phi| = 0.08$.