Supporting Information

The two-positron gluic bond as a manifestation of 'super' van der Waals interactions

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R_{HH}	DMC	MC-HF	R_{HH}	DMC	MC-HF
3.2	-1.3107	-1.1127	8.4	-1.3351	-1.1736
3.6	-1.3165	-1.1248	8.6	-1.3344	-1.1726
4.0	-1.3229	-1.1370	8.8	-1.3333	-1.1715
4.4	-1.3290	-1.1478	9.0	-1.3324	-1.1704
4.8	-1.3337	-1.1567	9.2	-1.3317	-1.1693
5.2	-1.3370	-1.1637	9.4	-1.3310	-1.1682
5.6	-1.3392	-1.1690	9.6	-1.3301	-1.1670
5.9	-1.3399	-1.1720	9.8	-1.3294	-1.1659
6.0	-1.3401	-1.1728	10.0	-1.3286	-1.1648
6.1	-1.3403	-1.1735	10.2	-1.3280	-1.1638
6.2	-1.3404	-1.1742	10.4	-1.3271	-1.1627
6.3	*-1.3405*	-1.1747	10.6	-1.3266	-1.1618
6.4	-1.3404	-1.1752	10.8	-1.3258	-1.1609
6.5	-1.3404	-1.1756	11.0	-1.3253	-1.1601
6.6	-1.3404	-1.1760	11.2	-1.3246	-1.1594
6.7	-1.3402	-1.1763	11.4	-1.3242	-1.1587
6.8	-1.3401	-1.1765	11.6	-1.3235	-1.1582
6.9	-1.3398	-1.1767	11.8	-1.3231	-1.1578
7.2	-1.3392	*-1.1769*	12.0	-1.3224	-1.1574
7.6	-1.3379	-1.1764	12.2	-1.3220	-1.1570
8.0	-1.3365	-1.1753	12.4	-1.3217	-1.1567
8.2	-1.3357	-1.1745	12.6	-1.3213	-1.1564

* To compute the bond dissociation energies from the total energies, the following data have been employed: For PsH, DMC and MC-HF/[QZ:QZ] total energies are -0.78920 and -0.66617 Hartree, respectively, whereas for H^-, DMC and MC-HF/[QZ:QZ] total energies are -0.52775 and -0.48781 Hartree, respectively.

Table S2 Total energies of $(PsH)_2$ as a function of the inter-proton distance computed at the DMC and MC-HF/[QZ:QZ] levels of theory for the singlet electronic and positronic spin states. The statistical errors of the QMC-derived energies are always below 10^{-4} Hartree. All values are given in atomic units.*

R_{HH}	DMC	MC-HF	R_{HH}	DMC	MC-HF
3.6	-1.5584	-1.2890	9.6	-1.5808	-1.3326
4.0	-1.5695	-1.3009	9.8	-1.5804	--
4.4	-1.5782	-1.3104	10.0	-1.5802	-1.3326
4.8	-1.5837	-1.3177	10.2	-1.5799	--
5.2	-1.5867	-1.3230	10.4	-1.5798	-1.3325
5.6	-1.5884	-1.3267	10.6	-1.5796	--
5.8	-1.5888	--	10.8	-1.5794	-1.3325
6.0	*-1.5888*	-1.3292	11.0	-1.5793	--
6.2	-1.5885	--	11.2	-1.5792	-1.3325
6.4	-1.5883	-1.3308	11.4	-1.5791	--
6.6	-1.5880	--	11.6	-1.5790	-1.3325
6.8	-1.5875	-1.3318	11.8	-1.5789	--
7.0	-1.5870	--	12.0	-1.5788	-1.3325
7.2	-1.5865	-1.3323	12.2	-1.5788	--
7.4	-1.5859	--	12.4	-1.5788	--
7.6	-1.5854	-1.3326	12.6	-1.5787	--
7.8	-1.5847	--	12.8	-1.5786	--
8.0	-1.5841	-1.3327	13.0	-1.5786	--
8.2	-1.5836	-1.3327	13.2	-1.5786	--
8.3	--	*-1.3327*	13.4	-1.5786	--
8.4	-1.5831	-1.3327	13.6	-1.5785	--
8.6	-1.5826	-1.3327	13.8	-1.5785	--
8.8	-1.5822	-1.3327	14.0	-1.5785	--
9.0	-1.5817	--	14.2	-1.5785	--
9.2	-1.5814	-1.3327	14.4	-1.5785	--
9.4	-1.5810	--			

* To compute the bond dissociation energies from the total energies, the following data have been employed for PsH : DMC and MC-HF/[QZ:QZ] total energies are -0.78920 and -0.66617 Hartree, respectively.

Table S3 Total energies of $(PsH)_2$ computed using the VMC method, and employing Heitler and London's wavefunction, denoted as VMC/HL (see the main text for details), as a function of the inter-proton distance, for the singlet electronic and positronic spin states. The statistical errors of the VMC-derived energies are always equal to or below 10^{-4} Hartree. All values are given in atomic units.

R_{HH}	VMC	R_{HH}	VMC
4.0	-1.5288	9.6	-1.5732
4.4	-1.5448	10.0	-1.5731
4.8	-1.5559	10.4	-1.5730
5.2	-1.5630	10.8	-1.5730
5.6	-1.5676	11.2	-1.5730
6.0	-1.5704	11.6	-1.5729
6.4	-1.5722	12.0	-1.5729
6.8	-1.5732	12.4	-1.5729
7.2	-1.5737	12.8	-1.5728
7.6	-1.5737	13.2	-1.5728
8.0	*-1.5738*	13.6	-1.5728
8.4	-1.5735	14.0	-1.5727
8.8	-1.5735	14.4	-1.5727
9.2	-1.5734	14.8	-1.5727

* To compute the bond dissociation energies from the total energies, the following data have been employed *PsH* : the VMC total energy is -0.78630 Hartree.

Table S4 The interatomic correlation energies (see the main text for definition) computed for the ground state $(PsH)_2$ as a function of the inter-proton distance. All values are given in atomic units.*

R_{HH}	$\Delta E^{corr}(R)$	R_{HH}	$\Delta E^{corr}(R)$
6.0	-0.0135	9.2	-0.0027
6.4	-0.0114	9.6	-0.0021
6.8	-0.0097	10.0	-0.0016
7.2	-0.0081	10.4	-0.0012
7.6	-0.0067	10.8	-0.0009
8.0	-0.0054	11.2	-0.0006
8.4	-0.0043	11.6	-0.0005
8.8	-0.0034	12.0	-0.0003

* The employed correlation energy of PsH is 0.12302 Hartree.

Table S5 The three contributions to the interatomic correlation energy computed at the MC-MP2 level (see the main text for details), for the ground state of $(PsH)_2$ as a function of the inter-proton distance. All values are given in atomic units.*

R_{HH}	$\Delta E_{ee}^{corr}(R)$	$\Delta E_{ep}^{corr}(R)$	$E_{pp}^{corr}(R)$
5.2	-0.0026	-0.0133	-0.0164
5.6	-0.0020	-0.0110	-0.0147
6.0	-0.0015	-0.0088	-0.0127
6.4	-0.0012	-0.0068	-0.0106
6.8	-0.0009	-0.0052	-0.0086
7.2	-0.0007	-0.0039	-0.0068
7.6	-0.0005	-0.0029	-0.0053
8.0	-0.0004	-0.0021	-0.0041
8.4	-0.0003	-0.0015	-0.0031
8.8	-0.0002	-0.0011	-0.0024
9.2	-0.0002	-0.0008	-0.0018
9.6	-0.0001	-0.0006	-0.0013
10.0	-0.0001	-0.0004	-0.0010
10.4	-0.0001	-0.0003	-0.0007
10.8	-0.0001	-0.0002	-0.0006
11.2	0.0000	-0.0002	-0.0004
11.6	0.0000	-0.0002	-0.0003
12.0	0.0000	-0.0001	-0.0003
12.4	0.0000	-0.0001	-0.0002
12.8	0.0000	-0.0001	-0.0002
13.2	0.0000	-0.0001	-0.0001
13.6	0.0000	-0.0001	-0.0001
14.0	0.0000	-0.0001	-0.0001
14.4	0.0000	0.0000	-0.0001

* The used electron-electron and electron-positron correlation energies of PsH are 0.02884 and 0.03633 Hartree, respectively.