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Title:	Evidence for reverse core-shell phase separation in mixed parahydrogen/orthodeuterium clusters with an ionic impurity
Authors:	Batra, N. (/jspui/browse?type=author&value=Batra%2C+N.)
Keywords:	Hydrogen clusters Path-integral molecular dynamics Quantum structural transition
Issue Date:	2018
Publisher:	Elsevier B.V.
Citation:	Chemical Physics Letters, 692, pp. 416-420
Abstract:	Using a flexible polarizable potential, the stable structures of H-(H ₂) _n (D ₂) _p clusters with fixed total size n+p=32 have been investigated by means of path-integral molecular dynamics simulations as a function of composition. The most stable phase is found to be reverse core-shell, in which the heavier deuterium molecules reside outside. This result contrasts with neutral clusters, in which deuterium preferentially occupies internal sites. This purely quantum effect is interpreted to originate from the significant weakening of hydrogen covalent bonds in the vicinity of the ionic impurity and its lowering of zero-point energy that affects H ₂ more than D ₂
Description:	Only IISERM authors are available in the record.
URI:	https://www.sciencedirect.com/science/article/pii/S000926141731151X (https://www.sciencedirect.com/science/article/pii/S000926141731151X) http://hdl.handle.net/123456789/2177 (http://hdl.handle.net/123456789/2177)
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