**Supplementary material (Table S1 with supporting references):**

**Table S1:** Summary of diatomic dications and trications that we have detected recently at Arizona State University with either high-current 17 keV $^{16}O^-$ or 8 keV $^{40}Ar^+$ ion beam sputtering of various samples (without additional gas flooding) [5,6,7].

(**Labels in bold** below refer to ion species that apparently had not been observed previously.

Underlined labels refer to ion species that have been studied theoretically previously. The present work includes calculations of the molecular systems listed below in (i) and (ii).)

(i) Results on oxygen-containing diatomic trications shown in the present work:
$NbO^{3+}$ [8,9,10,11] (Fig.4), $HfO^{3+}$ [12] (Fig.6), **$ReO^{3+}$** (Fig.2).

(ii) Results on oxygen-containing diatomic dications shown in the present work:
$NbO^{2+}$ [13,9,10,11] (Fig.3), $HfO^{2+}$ [14,15] (Fig.5), **$ReO^{2+}$** (Fig.1).

(iii) Results on oxygen-containing diatomic dications reported in ref. [6]:
$\underline{BeO}^{2+}$ [16,17,6], $CrO^{2+}$ [18,19,20,21], **$\underline{GaO}^{2+}$** [22,23], $AsO^{2+}$ [24,25], **$AgO^{2+}$**, **$SbO^{2+}$**.

(iv) Other oxygen-containing diatomic dications [5]:
**$\underline{MgO}^{2+}$** [26(a),26(c)], $\underline{AlO}^{2+}$ [27,28,29,30,31,32], $\underline{SiO}^{2+}$ [33,34,32(b)], $\underline{PO}^{2+}$ [35,36,37,38], $\underline{ClO}^{2+}$ [39], *$TiO^{2+}$* [40,41,42,43,29,44,45], $\underline{VO}^{2+}$ [46,47,48,21(c)], $MnO^{2+}$ [49,50], $CuO^{2+}$ [51,52,53,54,55,56,57], $ZnO^{2+}$ [13(a),58], $GeO^{2+}$ [59], **$\underline{SeO}^{2+}$** [60(a),60(b)], **$\underline{BrO}^{2+}$** [60(c)], ***$SrO^{2+}$***, *$YO^{2+}$* [61,52,53,62,63,55,32(c)], *$ZrO^{2+}$* [40,64,32(c)], $MoO^{2+}$ [13(a),59(a), 65,61,66,67(a)], $RuO^{2+}$ [68,69,33(d)], $CdO^{2+}$ [70,50], $InO^{2+}$ [71(a)], $\underline{SnO}^{2+}$ [61,71], $\underline{TeO}^{2+}$ [70,60(a)], **$IO^{2+}$**, *$BaO^{2+}$* [54,63], *$PrO^{2+}$* [61], ***$NdO^{2+}$*, *$SmO^{2+}$***, *$EuO^{2+}$* [54,56], *$GdO^{2+}$* [56, 72], *$TbO^{2+}$* [61,73], ***$DyO^{2+}$***, ***$HoO^{2+}$*, *$ErO^{2+}$*, *$TmO^{2+}$*, *$YbO^{2+}$***, $LuO^{2+}$ [72(a)]**,** $WO^{2+}$ [16,61, 67], $PtO^{2+}$ [74,29], $AuO^{2+}$ [8], **$TlO^{2+}$**, **$PbO^{2+}$**, $BiO^{2+}$ [61], $\underline{UO}^{2+}$ [61,75,76,77,78,79].

(v) Sulfur-containing diatomic dications [5]: **$MgS^{2+}$, $AsS^{2+}$**, **$PbS^{2+}$**.

(vi) Nitrogen-containing diatomic dications [5]: **SiN$^{2+}$**, **ClN$^{2+}$** [80,81,39(b)], *VN$^{2+}$* [82, 21(c)], GaN$^{2+}$ [83,21(d),32(e)]**,** **BrN$^{2+}$** [60(c)]**,** MoN$^{2+}$ [84].

(vii) Chlorine-metal diatomic dications [5]: MgCl$^{2+}$ [85,86], ***CaCl$^{2+}$*** [87,88], **CrCl$^{2+}$**, FeCl$^{2+}$ [89], **NiCl$^{2+}$, ZnCl$^{2+}$**, *SrCl$^{2+}$* [90], **PdCl$^{2+}$**, **CdCl$^{2+}$,** **SnCl$^{2+}$** [71(b)]**,** *BaCl$^{2+}$* [90], ***CeCl$^{2+}$*****,** ***YbCl$^{2+}$***, **PbCl$^{2+}$**.

(viii) Fluorine-metal diatomic dications and tricications [5]: **ZrF$^{3+}$** [1], *MgF$^{2+}$* [26(a),26(b),86], *CaF$^{2+}$* [91, 88(b)], *TiF$^{2+}$* [1], ***FeF$^{2+}$***, **NiF$^{2+}$**, ***ZrF$^{2+}$*** [1], ***SnF$^{2+}$*** [71(b)]**,** ***NdF$^{2+}$***.

(ix) Iodine-metal diatomic dications [5] **CaI$^{2+}$** [88], *BaI$^{2+}$* [90,92(a)].

(x) Hydrogen-containing diatomic dications [5]: ***CaH$^{2+}$*** [92(b),88(b)], ***SrH$^{2+}$***, **WH$^{2+}$**.

(xi) Homonuclear diatomic dications [7,5]: **Zn$_2^{2+}$** [93], **Zr$_2^{2+}$**, **Cd$_2^{2+}$** [94,93(b)], **Hf$_2^{2+}$, W$_2^{2+}$** [95], **Pt$_2^{2+}$** [96,95,97,7].

(xii) Other heteronuclear diatomic dications [5]: SiC$^{2+}$ [100,45(c)], **CaSi$^{2+}$** [88(b)]**,** **CaP$^{2+}$** [88(b)]**,** **SiGe$^{2+}$**, MgBr$^{2+}$ [90], *CaBr$^{2+}$* [90,88], **CuZn$^{2+}$** [101]**,** **AsFe$^{2+}$**.

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Additional note: Several of the above heteronuclear diatomic dications are predicted to be thermodynamically stable molecules (shown above as *labels in italics*), based on a comparison of the first and second ionization energies of their respective atomic fragments [102,90,6].

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