I think that a specie is an ordered sequence of DNA (or virus RNA) genes (genotype); for example for the Pelagibacter ubique:

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If there is a difference in the ordered sequence (by number, by gene value or by permutation of genes) then the species are different.

An hybrid between species is ever possible, but the probability of embryo survival is related to the differences in the ordered sequence of genes: the lack of overlapping of genes, in the meiosis, causes the lack of coding of molecules essential for life, so that different in the sequences do not make survive the embryos (population are reproductively isolated).

The genotype determines the phenotype, so that the taxonomy of a species using the observed characters is an approximation of the gene sequencing (this is more true for elementary organisms like bacteria).

If new life will be expressed as Artificial Intelligence, then the soubroutine of the program (coded as genes), and the soubroutine tree could be the genotype of the artificial life.